IUPAC-NIST Solubility Data Series. 99. Solubility of Benzoic Acid and Substituted Benzoic Acids in Both Neat Organic Solvents and Organic Solvent Mixtures

William E. Acree, Jr.[a)]

Department of Chemistry, University of North Texas, Denton, Texas 76203, USA

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Solubility data are compiled and reviewed for benzoic acid and 63 substituted benzoic acids dissolved in neat organic solvents and well-defined binary and ternary organic solvent mixtures. The compiled solubility data were retrieved from the published chemical and pharmaceutical literature covering the period from 1900 to the beginning of 2013. © *2013 AIP Publishing LLC.* [http://dx.doi.org/10.1063/1.4816161]

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CONTENTS

[a)] Electronic mail: acree@unt.edu.

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List of Tables

1. Preface

1.1. Scope of this volume

This volume reviews experimentally determined solubility data for benzoic acid and 63 substituted benzoic acids dissolved in neat organic solvents and well-defined binary and ternary organic solvent mixtures retrieved from the published chemical and pharmaceutical literature covering the period from 1900 to the end of 2012. Solubility data are compiled and critically reviewed for benzoic acid, 2-acetoxybenzoic acid, 4-acetoxybenzoic acid, 4-acetylbenzoic acid, 2-aminobenzoic acid, 3-aminobenzoic acid, 4-aminobenzoic acid, 4-amino-2-hydroxybenzoic acid, 5-amino-2-hydroxybenzoic acid, 1,2-benzenedicarboxylic acid, 1,3-benzenedicarboxylic acid, 1,4-benzenedicarboxylic acid, 1,3,5-benzenetricarboxylic acid, 2-bromobenzic acid, 3-bromobenzoic acid, 4-bromobenzoic acid, 2-chlorobenzoic acid, 3-chlorobenzoic acid, 4-chlorobenzoic acid, 2-chloro-5-nitrobenzoic acid, 4-chloro-3,5-dinitrobenzoic acid, 4-chloro-3-nitrobenzoic acid, 4-cyanobenzoic acid, 3,5-diaminobenzoic acid, 2,4-dichlorobenzoic acid, 3,5-dichlorobenzoic acid, 2,4-dihydroxybenzoic acid, 2,5-dihydroxybenzoic acid, 2,6-dihydroxybenzoic acid, 3,4-dihydroxybenzoic acid, 2,6-dimethoxybenzoic acid, 3,4-dimethoxybenzoic acid, 3,5-dimethoxybenzoic acid, 3-(dimethylamino)benzoic acid, 4-(dimethylamino)benzoic acid, 3,4-dimethylbenzoic acid, 2,4-dinitrobenzoic acid, 3,5-dinitrobenzoic acid, 3,5-dinitro-2-methylbenzoic acid, 2-fluorobenzoic acid, 3-fluorobenzoic acid, 4-fluorobenzoic acid, 4-formylbenzoic acid, 2-hydroxybenzoic acid, 3-hydroxybenzoic acid, 4-hydroxybenzoic acid, 2-hydroxy-3-methylbenzoic acid, 2-hydroxy-4-methylbenzoic acid, 2-hydroxy-5-methylbenzoic acid, 3-hydroxy-4-methylbenzoic acid, 4-hydroxy-3-methoxybenzoic acid, 4-hydroxy-3-methylbenzoic acid, 4-iodobenzoic acid, 2-methoxybenzoic acid, 3-methoxybenzoic acid, 4-methoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 4-methylbenzoic acid, 2-nitrobenzoic acid, 3-nitrobenzoic acid, 4-nitrobenzoic acid, and 3-nitro-1,2-benzenedicarboxylic acid. Aqueous systems and inorganic systems (namely supercritical carbon dioxide) are not included in this volume. Readers wishing solubility data for aqueous and inorganic systems are referred to Vol. 90 in the IUPAC-NIST Solubility Data Series,[1,2] which dealt with the solubility of hydroxybenzoic acid derivatives in binary, ternary and multicomponent systems. Here one will find solubility data for 2-hydroxybenzoic acid, 3-hydroxybenzoic acid and 4-hydroxybenzoic acid, as well as solubility data for several 4-hydroxybenzoate alkyl esters (parabens) and hydroxybenzoic acid salts. As an informational note, Vol. 90 contains solubility data for the three hydroxybenzoic acids dissolved in organic solvents. The solubility data reported in the current volume for organic solvents are slightly more extensive and include references that were either published after or overlooked in the preparation of the earlier volume.

Several substituted benzoic acids and benzoic acid derivatives exhibit therapeutic properties. For example, 2-hydroxybenzoic acid (commonly known as salicylic acid) is a nonsteroidal anti-inflammatory drug (NSAID) used to alleviate aches and pains, and is a key ingredient in many “over-the-counter” and prescription skin-care products for the treatment of acne, psoriasis, corns, warts, calluses, and seborrhoeic dermatitis. Salicylic acid is also an ingredient in shampoos added to control dandruff and dry scalp. Its methyl ester, methyl salicylate, can be applied topically as a liniment to relieve joint and muscle pains. 2-Acetoxybenzoic acid (aspirin) is widely used and prescribed in the treatment of a number of medical conditions, including fever, muscle aches and pains, rheumatoid arthritis, and pericarditis. 2-Acetoxybenzoic acid has also been used long-term, at low doses, to help prevent heart attacks, strokes, and blood clot formation in individuals at high risk of developing blood clots. 4-Aminobenzoic acid is one of the components of the folic acid molecule, and is an effective chemical sunscreen (absorbs ultraviolet and visible sun light) when applied topically. 4-Aminosalicylic acid is an antibiotic, prescribed alone or in combination with other drugs, in the treatment of tuberculosis. 5-Amino-2-hydroxybenzoic acid is a drug used for treating *ulcerative colitis*, which is a chronic inflammation of the large intestine. 4-Hydroxy-3-methoxybenzoic acid has been used as a flavoring agent for many years, and is known for its anthelmintic properties.

1.2. Concentration units for nonelectrolyte solutions

Composition of a liquid nonelectrolyte solution can be expressed in a variety of ways, as (1) the ratio of the number of moles of one component to the number of moles of a second component, n_1/n_2, etc., (2) molar concentration

$$c_i = [i] = \frac{n_i}{V} \qquad \text{SI base units : mol dm}^{-3}, \tag{1}$$

(3) mole fraction

$$x_i = \frac{n_i}{n_1 + n_2 + \,.....\, + n_i + \,\ldots.}, \tag{2}$$

or (4) volume fraction

$$\phi_i = \frac{n_i\, V_i}{n_1\, V_1 + n_2\, V_2 + \,.....\, + n_i\, V_i + \,\ldots.}. \tag{3}$$

Strictly speaking, the true volume of a real solution is not equal to the sum of the volumes of the individual components but is the mole-fraction sum of partial volumes, which for a ternary solution is $V = x_1 V_1 + x_2 V_2 + x_3 V_3$. For purposes of this study, volume fractions are defined in terms of the molar volumes of the pure unmixed components, $V_{\mathrm{m},i}$ (molar mass of component i divided by density of component i)

$$\varphi_i = \frac{n_i\, V_{\mathrm{m},i}}{n_1\, V_{\mathrm{m},1} + n_2\, V_{\mathrm{m},2} + \,.....\, + n_i\, V_{\mathrm{m},i} + \,\ldots.}, \tag{4}$$

as this quantity serves as an input parameter in expressions for estimating solubilities in mixed solvents since it requires no *a priori* knowledge concerning volumetric behavior. Solute solubilities can be found in the chemical literature in terms of any of the aforementioned concentration variables, or as molality, m_i, which is the number of moles of solute i divided by the mass of the solvent

$$m_i = \frac{n_i}{n_{\text{solvent}} M_{\text{solvent}}} \qquad \text{SI base units : mol kg}^{-1}, \tag{5}$$

where M_{solvent} is the molar mass of the solvent.

1.3. Procedures used in critical evaluation of published solubility data

Procedures used in the critical evaluation of published solubility data for crystalline nonelectrolytes dissolved in organic monosolvents and organic solvent mixtures depend to a large extent on the quantity and type of data to be evaluated. In those instances where independent experimental measurements exist, one can compute the mean value and standard deviation for each set of replicate values (or set of values) differing from the rest. This type of analysis will be limited primarily to the neat mono-solvents as published data for binary and ternary solvent mixtures are relatively scarce compared to solubility data for solutes dissolved in single solvent systems. Given the scarcity of binary solvent and ternary solvent solubility data, researchers have tended to perform measurements on new mixtures as opposed to repeating measurements on already studied mixtures, even if measured at different temperatures.

Published solubility data may be found for a given solute-solvent system measured at several different temperatures. The temperature variation can be critically evaluated using standard thermodynamic relationships based on the ideal mole fraction solubility of a solid solute, $x_1^{\text{ideal soly}}$ in a liquid solvent[3]

$$-\ln x_1^{\text{ideal soly}} = \frac{\Delta H_1^{\text{fus}}}{RT}\left[1 - \frac{T}{T_{\text{mp}}}\right] + \frac{\Delta C_{p,1}}{R}\left(\frac{T_{\text{mp}} - T}{T}\right) + \frac{\Delta C_{p,1}}{R}\ln\left(\frac{T_{\text{mp}}}{T}\right), \tag{6}$$

where ΔH_1^{fus} is the standard molar enthalpy of fusion of the solute at its normal melting point temperature, T_{mp}, $\Delta C_{p,1}$ is the difference in the molar heat capacities of the liquid and crystalline forms of the solute (i.e., $\Delta C_{p,1} = C_{p,\text{liquid}} - C_{p,\text{solid}}$) and R is the universal gas constant. Through suitable algebraic manipulations, Eq. (6) can be rearranged to give

$$\ln x_1^{\text{ideal soly}} = \left[\frac{\Delta H_1^{\text{fus}}}{R\,T_{\text{mp}}} + \frac{\Delta C_{p,1}}{R}(1 + \ln T_{\text{mp}})\right] - \left(\frac{\Delta H_1^{\text{fus}}}{R} + \frac{\Delta C_{p,1} T_{\text{mp}}}{R}\right)\frac{1}{T} + \frac{\Delta C_{p,1}}{R}\ln T, \tag{7}$$

which has the generalized mathematical form of

$$\ln x_1 = A + \frac{B}{T} + C \ln T. \tag{8}$$

Though derived for an ideal solution, Eq. (8) has been used successfully to describe solute solubility in many nonideal solutions. The equation is commonly referred to as the Modified Apelblat equation in the published literature.

The λh model, developed by Buchowski *et al.*,[4,5] is

$$\ln\left[1 + \frac{\lambda(1 - x_1)}{x_1}\right] = \lambda\, h\left(\frac{1}{T} - \frac{1}{T_{\text{mp}}}\right), \tag{9}$$

a second popular mathematical representation for describing how the mole-fraction solubility varies with solution temperature. In Eq. (9), T and T_{mp} refer to the solution temperature and melting-point temperature of the solute, respectively. The two model parameters, λ and h, are determined by least-squares analyses using the measured mole-fraction solubilities. Experimental solubility data are considered to be internally consistent if the measured x_i values can be accurately described by Eqs. (8) and/or (9).

Solution models have been used with success to rationalize the solubility behavior of a given solute molecule in a series of organic solvents. Of the models developed in recent years, the general solvation parameter developed by Abraham and coworkers[6–14] is probably the most widely used approach in correlating the solubilities of substituted benzoic acids. The model is based on two linear free energy relationships describing solute transfer between two immiscible phases. The first expression quantifies solute transfer between two condensed phases

$$\log_{10}(SR \text{ or } P) = c_{\text{p}} + e_{\text{p}}\cdot E + s_{\text{p}}\cdot S + a_{\text{p}}\cdot A + b_{\text{p}}\cdot B + v_{\text{p}}\cdot V, \tag{10}$$

and the second expression involves solute transfer from the gas phase

$$\log_{10}(GSR \text{ or } K) = c_{\text{k}} + e_{\text{k}}\cdot E + s_{\text{k}}\cdot S + a_{\text{k}}\cdot A + b_{\text{k}}\cdot B + l_{\text{k}}\cdot L, \tag{11}$$

where P is the water-to-organic solvent partition coefficient or nonpolar organic solvent-to-polar organic solvent partition coefficient, and K is the gas-to-organic solvent partition coefficient. For solubility predictions, the Abraham model uses the solubility ratio which is given by the ratio of the molar solubilities of the solute in the organic solvent, $c_{1,\text{S}}^{\text{sat}}$, and in water, $c_{1,\text{W}}^{\text{sat}}$ (i.e., $SR = c_{1,\text{S}}^{\text{sat}} / c_{1,\text{W}}^{\text{sat}}$). The gas phase solubility ratio is similarly calculated as the molar solubility in the organic solvent divided by the solute gas phase concentration (i.e., $GSR = c_{1,\text{S}}^{\text{sat}}/c_{1,\text{G}}$), the latter value calculable from the solute vapor pressure above the solid at the solution temperature.

The dependent variables in Eqs. (10) and (11) are solute descriptors as follows: E is the solute excess molar refraction (in units of cm^3 mol^{-1}/10), S refers to the solute dipolarity/polarizability, A and B represent the overall solute hydrogen bond acidity and basicity, V denotes the solute's McGowan characteristic molecular volume (in units of cm^3 mol^{-1}/100), and L is the logarithm of the gas-to-hexadecane partition coefficient measured at 298 K. The lower-case regression coefficients and constants (c_{p}, e_{p}, s_{p}, a_{p}, b_{p}, v_{p}, c_{k}, e_{k}, s_{k}, a_{k}, b_{k}, and l_{k}) in Eqs. (10) and (11) are obtained by multiple linear regression analysis of experimental partition coefficient data and solubility ratios for a specific biphasic system. To date Abraham model correlations have been developed for predicting the solubility of crystalline nonelectrolytes in more than 70 different organic solvents,[15–22] for predicting the water-to-organic solvent and gas-to-organic solvent partition coefficient for more than 70 different biphasic systems,[15–24] and for predicting the partition coefficients of organic vapors and gaseous solutes into aqueous micellar solvent media,[25,26] into humic acid,[27] and into various body tissues and fluids.[28–34] Each of the aforementioned predictions requires *a priori* knowledge of the compound's solute descriptors as input parameters.

Equation (10) correlates experimental partition coefficients and/or solubility ratios, and for select organic solvents both "dry" and "wet" equation coefficients have been reported. For solvents that are partially miscible with water, such as 1-pentanol and butyl ethanoate, solubility ratios calculated as the molar solute solubility in the organic solvent divided by the solute's aqueous molar solubility are not the same as those obtained from direct partition between water (saturated with the organic solvent) and organic solvent (saturated with water). Care must be taken not to confuse the two sets of transfer process. There should be no confusion in the case of solvents that are fully miscible with water, such as ethanol. Only one set of equation coefficients has been published, and the dependent variable is the logarithm of the solubility ratio. And for solvents that are "almost" completely immiscible with water, such as alkylbenzenes (benzene, toluene, etc.) and chloroalkanes (1,2-dichloroethane, chloroform), there should be no confusion because the solubility ratio [see Eq. (3)] will be nearly identical to the practical partition coefficient.

Applicability of the Abraham solvation parameter model is fairly straightforward. One starts with the set of equations that have been obtained for the ratio of the molar solubilities of the solute in the organic solvent and in water (i.e., $SR = c_{1,\mathrm{S}}^{\mathrm{sat}} \,/\, c_{1,\mathrm{W}}^{\mathrm{sat}}$). Table 1 lists the coefficients in Eq. (10) for transfer processes that shall be considered in the present volume. It is noted that coefficients are periodically revised when additional experimental data become available. Thus, if $c_{1,\mathrm{W}}^{\mathrm{sat}}$ is known, predicted $\log_{10} SR$ values based upon Eq. (10) will lead to predicted molar solubilities in organic solvents through $SR = c_{1,\mathrm{S}}^{\mathrm{sat}} \,/\, c_{1,\mathrm{W}}^{\mathrm{sat}}$.

Solubilities in organic solvents can also be predicted and correlated with Eq. (11). Listed in Table 2 are the equation coefficients that have been previously determined for the gas phase solubility ratio, $GSR = c_{1,\mathrm{S}}^{\mathrm{sat}}/c_{1,\mathrm{G}}$. Predicted $\log_{10} GSR$ values can also be converted to saturation molar solubilities, provided that the saturated vapor pressure above the crystalline solute at 298.15 K, VP°, is known. VP° is transformed into the solute's gas phase molar concentration, $c_{1,\mathrm{G}}$, which is then used to calculate the respective gas-to-water and gas-to-solvent partition coefficients, GSR_W and GSR_S:

$$GSR_\mathrm{W} = c_{1,\mathrm{W}}^{\mathrm{sat}}/c_{1,\mathrm{G}}^{\mathrm{sat}} \quad \text{or} \quad \log_{10} GSR_\mathrm{W} = \log_{10} c_{1,\mathrm{W}}^{\mathrm{sat}} - \log_{10} c_{1,\mathrm{G}}, \tag{12}$$

$$GSR_\mathrm{S} = K_\mathrm{S} = c_{1,\mathrm{S}}^{\mathrm{sat}}/c_{1,\mathrm{G}} \quad \text{or} \quad \log_{10} GSR_\mathrm{S} = \log_{10} c_{1,\mathrm{S}}^{\mathrm{sat}} - \log_{10} c_{1,\mathrm{G}}. \tag{13}$$

An estimated value of $c_{1,\mathrm{G}}$ can be assumed in the preliminary calculations if an experimental vapor pressure cannot be located in the published literature for the solute at 298.15 K. The value can be adjusted if necessary in order to reduce the $\log_{10} GSR$ deviations, and to make the $\log_{10} SR$ and $\log_{10} GSR$ computations internally consistent as discussed in several previous publications.

Three specific conditions must be met in order to use the Abraham solvation parameter model to predict saturation solubilities. First, the same solid phase must be in equilibrium with the saturated solutions in the organic solvent and in water (i.e., there should be no solvate or hydrate formation). Second, the secondary medium activity coefficient of the solid in the saturated solutions must be unity (or near unity). This condition generally restricts the method to those solutes that are sparingly soluble in water and nonaqueous solvents. Finally, for solutes that are ionized in aqueous solution, $c_{\mathrm{A,water}}$ refers to the solubility of the neutral monomeric form. In the case of substituted benzoic acids, this will limit the model to solvents such as alcohols, short alkyl chain ethers, alkyl alkanoates and propylene carbonate. Carboxylic acids are known to dimerize in alkane and nonpolar aromatic solvents, and the solute descriptors that have been calculated for the benzoic acid derivatives pertain to the monomeric form. The second restriction involving the secondary medium activity coefficient may not be as important as initially believed. The Abraham solvation parameter model has shown remarkable success in correlating the solubility of several very soluble crystalline solutes. For example, Eqs. (10) and (11) described the molar solubility of benzil in 24 organic solvents to within overall standard deviations of 0.124 and 0.109 $\log_{10}$ units, respectively.[35] Standard deviations for acetylsalicylic acid dissolved in 13 alcohols, 4 ethers, and ethyl ethanoate were 0.123 and 0.138 $\log_{10}$ units.[12] Benzil[35] and acetylsalicylic acid[12] exhibited solubilities exceeding 1 molar in several of the organic solvents studied. In the case of acetylsalicylic acid, it could be argued that the model's success relates back to when the equation coefficients were originally calculated for the dry solvents. The databases used in the regression analyses contained very few carboxylic acid solutes (benzoic acid, 2-hydroxybenzoic acid, and 4-hydroxybenzoic acid). Most of the experimental data for carboxylic acids and other very acidic solutes was in the form of saturation solubilities, which were also in the 1–3 molar range. Such arguments do not explain why Eqs. (10) and (11) described the measured benzil solubility data. The benzil solubilities were measured after most of the equation coefficients were first determined.

Numerical values of solute descriptors exist for more than 5000 different organic and organometallic compounds, and if not readily available are easily calculable from measured partition coefficient and solubility data.[7,15,36,37] The McGowan volume solute descriptor, V, is calculated from the molecular formula and the number of chemical bonds in the solute as follows:[38]

$$V = \sum_i^{\mathrm{atoms}} n_i AV_i - 6.56\, n_{\mathrm{bonds}}, \tag{14}$$

where n_i and AV_i denote the number of atoms and atomic volume of element i in the solute molecule, respectively, and

TABLE 1. Abraham model equation coefficients describing solute transfer to an organic solvent from water [Eq. (10)]

Organic solvent	c_p	e_p	s_p	a_p	b_p	v_p
Dichloromethane	0.319	0.102	−0.187	−3.058	−4.090	4.324
Trichloromethane	0.191	0.105	−0.403	−3.112	−3.514	4.395
Tetrachloromethane	0.199	0.523	−1.159	−3.560	−4.594	4.618
1,2-Dichloroethane	0.183	0.294	−0.134	−2.801	−4.291	4.180
1-Chlorobutane	0.222	0.273	−0.569	−2.918	−4.883	4.456
Hexane	0.333	0.560	−1.710	−3.578	−4.939	4.463
Heptane	0.297	0.634	−1.755	−3.571	−4.946	4.488
Octane	0.241	0.690	−1.769	−3.545	−5.011	4.511
Decane	0.172	0.726	−1.750	−3.446	−4.496	4.489
Undecane	0.058	0.603	−1.661	−3.421	−5.120	4.619
Dodecane	0.114	0.668	−1.644	−3.545	−5.006	4.459
Hexadecane	0.087	0.667	−1.617	−3.587	−4.869	4.433
Cyclohexane	0.159	0.784	−1.678	−3.740	−4.929	4.577
Methylcyclohexane	0.246	0.782	−1.982	−3.517	−4.293	4.528
2,2,4-Trimethylpentane	0.318	0.555	−1.737	−3.677	−4.864	4.417
Benzene	0.142	0.464	−0.588	−3.099	−4.625	4.491
Toluene	0.125	0.431	−0.644	−3.002	−4.748	4.524
Ethylbenzene	0.093	0.467	−0.723	−3.001	−4.844	5.514
1,2-Dimethylbenzene	0.083	0.518	−0.813	−2.884	−4.821	4.559
1,3-Dimethylbenzene	0.122	0.377	−0.603	−2.981	−4.961	4.535
1,4-Dimethylbenzene	0.166	0.477	−0.812	−2.939	−4.874	4.532
Fluorobenzene	0.139	0.152	−0.374	−3.030	−4.601	4.540
Chlorobenzene	0.065	0.381	−0.521	−3.183	−4.700	4.614
Bromobenzene	−0.017	0.436	−0.424	−3.174	−4.558	4.445
Iodobenzene	−0.192	0.298	−0.308	−3.213	−4.653	4.588
Nitrobenzene	−0.152	0.525	0.081	−2.332	−4.494	4.187
Benzonitrile	0.097	0.285	0.059	−1.605	−4.562	4.028
Olive oil	−0.035	0.574	−0.798	−1.422	−4.984	4.210
Carbon disulfide	0.047	0.686	−0.943	−3.603	−5.818	4.921
Isopropyl myristate	−0.605	0.930	−1.153	−1.682	−4.093	4.249
Triolein	0.385	0.983	−2.083	−2.007	−3.452	4.072
Methanol	0.276	0.334	−0.714	0.243	−3.320	3.549
Ethanol	0.222	0.471	−1.035	0.326	−3.596	3.857
Propan-1-ol	0.139	0.405	−1.029	0.247	−3.767	3.986
Butan-1-ol	0.165	0.401	−1.011	0.056	−3.958	4.044
Pentan-1-ol	0.150	0.536	−1.229	0.141	−3.864	4.077
Hexan-1-ol	0.115	0.492	−1.164	0.054	−3.978	4.131
Heptan-1-ol	0.035	0.398	−1.063	0.002	−4.342	4.317
Octan-1-ol	−0.034	0.489	−1.044	−0.024	−4.235	4.218
Decan-1-ol	−0.058	0.616	−1.319	0.026	−4.153	4.279
Propan-2-ol	0.102	0.315	−1.020	0.532	−3.865	4.023
2-Methylpropan-1-ol	0.161	0.310	−1.069	0.183	−3.774	4.040
2-Butanol	0.194	0.383	−0.956	0.134	−3.606	3.829
2-Methylpropan-2-ol	0.197	0.136	−0.916	0.318	−4.031	4.112
3-Methylbutan-1-ol	0.123	0.370	−1.243	0.074	−3.781	4.208
2-Pentanol	0.115	0.455	−1.331	0.206	−3.745	4.201
Ethylene glycol	−0.270	0.578	−0.511	0.715	−2.619	2.729
2,2,2-Trifluoroethanol	0.395	−0.094	−0.594	−1.280	−1.274	3.088
1,1′-Oxybisethane	0.330	0.401	−0.814	−0.457	−4.959	4.320
Tetrahydrofuran	0.207	0.372	−0.392	−0.236	−4.934	4.447
Dioxane	0.098	0.350	−0.083	−0.556	−4.826	4.172
1,1′-Oxybisbutane	0.203	0.369	−0.954	−1.488	−5.426	4.508
2-Methoxy-2-methylpropane	0.376	0.264	−0.788	−1.078	−5.030	4.410
Methyl ethanoate	0.351	0.223	−0.150	−1.035	−4.527	3.972
Ethyl ethanoate	0.328	0.369	−0.446	−0.700	−4.904	4.150
Propyl ethanoate	0.288	0.363	−0.474	−0.784	−4.939	4.216
Butyl ethanoate	0.248	0.356	−0.501	−0.867	−4.973	4.281
Propanone	0.313	0.312	−0.121	−0.608	−4.753	3.942
Butanone	0.246	0.256	−0.080	−0.767	−4.855	4.148
Cyclohexanone	0.038	0.225	0.058	−0.976	−4.842	4.315
Propylene carbonate	0.004	0.168	0.504	−1.283	−4.407	3.421
Dimethylformamide	−0.305	−0.058	0.343	0.358	−4.865	4.486
Dimethylacetamide	−0.271	0.084	0.209	0.915	−5.003	4.557
Diethylacetamide	0.213	0.034	0.089	1.342	−5.084	4.088
Dibutylformamide	0.332	0.302	−0.436	0.358	−4.902	3.952
N-Methylpyrolidinone	0.147	0.532	0.225	0.840	−4.794	3.674

TABLE 1. Abraham model equation coefficients describing solute transfer to an organic solvent from water [Eq. (10)]—Continued

Organic solvent	c_p	e_p	s_p	a_p	b_p	v_p
N-Methyl-2-piperidone	0.056	0.332	0.257	1.556	−5.035	3.983
N-Formylmorpholine	−0.032	0.696	−0.062	0.014	−4.092	3.405
N-Methylformamide	0.114	0.407	−0.287	0.542	−4.085	3.471
N-Ethylformamide	0.220	0.034	−0.166	0.935	−4.589	3.730
N-Methylacetamide	0.090	0.205	−0.172	1.305	−4.589	3.833
N-Ethylacetamide	0.284	0.128	−0.442	1.180	−4.728	3.856
Formamide	−0.171	0.070	0.308	0.589	−3.152	2.432
Acetonitrile	0.413	0.077	0.326	−1.566	−4.391	3.364
Nitromethane	0.023	−0.091	0.793	−1.463	−4.364	3.460
Dimethylsulfoxide	−0.194	0.327	0.791	1.260	−4.540	3.361
Sulfolane (303 K)	0.000	0.147	0.601	−0.318	−4.541	3.290
Tributylphosphate	0.327	0.570	−0.837	−1.069	−4.333	3.919
Gas-water	−0.994	0.577	2.549	3.813	4.841	−0.869

n_{bonds} is the number of chemical bonds. The bond contribution is 6.56 $\text{cm}^3\ \text{mol}^{-1}$ for each bond, no matter whether single, double, or triple, to be subtracted. In other words, double and triple bonds count as one bond. Numerical values of AV_i for elements present in substituted benzoic acids are: $AV_C = 16.35\ \text{cm}^3\ \text{mol}^{-1}$; $AV_H = 8.71\ \text{cm}^3\ \text{mol}^{-1}$; $AV_N = 14.39\ \text{cm}^3\ \text{mol}^{-1}$; $AV_O = 12.43\ \text{cm}^3\ \text{mol}^{-1}$; $AV_F = 10.48\ \text{cm}^3\ \text{mol}^{-1}$; $AV_{Cl} = 20.95\ \text{cm}^3\ \text{mol}^{-1}$; $AV_{Br} = 26.21\ \text{cm}^3\ \text{mol}^{-1}$; $AV_I = 34.53\ \text{cm}^3\ \text{mol}^{-1}$; $AV_S = 22.91\ \text{cm}^3\ \text{mol}^{-1}$; and $AV_P = 24.87\ \text{cm}^3\ \text{mol}^{-1}$.

The numerical value of the excess molar refraction solute descriptor, E, is also fairly easy to calculate. It is defined as the molar refraction of the solute using McGowan's volume, MR_X, minus the molar refraction of an alkane

TABLE 2. Abraham model equation coefficients describing solute transfer to an organic solvent from gas phase [Eq. (11)]

Organic solvent	c_k	e_k	s_k	a_k	b_k	l_k
Oleyl alcohol	−0.268	−0.392	0.800	3.117	0.978	0.918
Dichloromethane	0.192	−0.572	1.492	0.460	0.847	0.965
Trichloromethane	0.157	−0.560	1.259	0.374	1.333	0.976
Tetrachloromethane	0.217	−0.435	0.554	0.000	0.000	1.069
1,2-Dichloroethane	0.017	−0.337	1.600	0.774	0.637	0.921
1-Chlorobutane	0.130	−0.581	1.114	0.724	0.000	1.016
Hexane	0.320	0.000	0.000	0.000	0.000	0.945
Heptane	0.284	0.000	0.000	0.000	0.000	0.950
Octane	0.219	0.000	0.000	0.000	0.000	0.960
Decane	0.159	0.000	0.000	0.000	0.000	0.972
Undecane	0.113	0.000	0.000	0.000	0.000	0.971
Dodecane	0.053	0.000	0.000	0.000	0.000	0.986
Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000
Cyclohexane	0.163	−0.110	0.000	0.000	0.000	1.013
Methylcyclohexane	0.318	−0.215	0.000	0.000	0.000	1.012
2,2,4-Trimethylpentane	0.264	−0.230	0.000	0.000	0.000	0.975
Benzene	0.107	−0.313	1.053	0.457	0.169	1.020
Toluene	0.085	−0.400	1.060	0.501	0.154	1.011
Ethylbenzene	0.059	−0.295	0.924	0.537	0.098	1.010
1,2-Dimethylbenzene	0.064	−0.296	0.934	0.647	0.000	1.010
1,3-Dimethylbenzene	0.071	−0.423	1.068	0.552	0.000	1.014
1,4-Dimethylbenzene	0.113	−0.302	0.826	0.651	0.000	1.011
Fluorobenzene	0.181	−0.621	1.432	0.647	0.000	0.986
Chlorobenzene	0.064	−0.399	1.151	0.313	0.171	1.032
Bromobenzene	−0.064	−0.326	1.261	0.323	0.292	1.002
Iodobenzene	−0.171	−0.192	1.197	0.245	0.245	1.002
Nitrobenzene	−0.295	0.121	1.682	1.247	0.370	0.915
Benzonitrile	−0.075	−0.341	1.798	2.030	0.291	0.880
Olive oil	−0.159	−0.277	0.904	1.695	−0.090	0.876
Carbon disulfide	0.101	0.251	0.177	0.027	0.095	1.068
Triolein	0.147	0.254	−0.246	1.520	1.473	0.918
Methanol	−0.039	−0.338	1.317	3.826	1.396	0.773
Ethanol	0.017	−0.232	0.867	3.894	1.192	0.846
Propan-1-ol	−0.042	−0.246	0.749	3.888	1.076	0.874
Butan-1-ol	−0.004	−0.285	0.768	3.705	0.879	0.890
Pentan-1-ol	−0.002	−0.161	0.535	3.778	0.960	0.900

TABLE 2. Abraham model equation coefficients describing solute transfer to an organic solvent from gas phase [Eq. (11)]—Continued

Organic solvent	c_k	e_k	s_k	a_k	b_k	l_k
Hexan-1-ol	−0.014	−0.205	0.583	3.621	0.891	0.913
Heptan-1-ol	−0.056	−0.216	0.554	3.596	0.803	0.933
Octan-1-ol	−0.147	−0.214	0.561	3.507	0.749	0.943
Decan-1-ol	−0.139	−0.090	0.356	3.547	0.727	0.958
Propan-2-ol	−0.062	−0.327	0.707	4.024	1.072	0.886
2-Methylpropan-1-ol	0.012	−0.407	0.670	3.645	1.283	0.895
Butan-2-ol	−0.017	−0.376	0.852	3.740	1.161	0.867
2-Methylpropan-2-ol	0.071	−0.538	0.818	3.951	0.823	0.905
3-Methylbutan-1-ol	−0.014	−0.341	0.525	3.666	1.096	0.925
2-Pentanol	−0.031	−0.325	0.496	3.792	1.024	0.934
Ethylene glycol	−0.887	0.132	1.657	4.457	2.325	0.565
2,2,2-Trifluoroethanol	−0.092	−0.547	1.339	2.213	3.807	0.645
1,1′-Oxybisethane	0.288	−0.347	0.775	2.985	0.000	0.973
Tetrahydrofuran	0.189	−0.347	1.238	3.289	0.000	0.982
Dioxane	−0.034	−0.354	1.674	3.021	0.000	0.919
1,1′-Oxybisbutane	0.165	−0.421	0.760	2.102	−0.664	1.002
2-Methoxy-2-methylpropane	0.278	−0.489	0.801	2.495	0.000	0.993
Methyl ethanoate	0.129	−0.447	1.675	2.625	0.213	0.874
Ethyl ethanoate	0.182	−0.352	1.316	2.891	0.000	0.916
Propyl ethanoate	0.165	−0.383	1.264	2.757	0.000	0.954
Butyl ethanoate	0.147	−0.414	1.212	2.623	0.000	0.954
Propanone	0.127	−0.387	1.733	3.060	0.000	0.866
Butanone	0.112	−0.474	1.671	2.878	0.000	0.916
Cyclohexanone	−0.086	−0.441	1.725	2.786	0.000	0.957
Propylene carbonate	−0.356	−0.413	2.587	2.207	0.455	0.719
Dimethylformamide	−0.391	−0.869	2.107	3.774	0.000	1.011
Dimethylacetamide	−0.308	−0.736	1.802	4.361	0.000	1.028
Diethylacetamide	−0.075	−0.434	1.911	4.801	0.000	0.899
Dibutylformamide	−0.002	−0.239	1.402	4.029	0.000	0.900
N-Methylpyrrolidinone	−0.128	−0.029	2.217	4.429	0.000	0.777
N-Methyl-2-piperidone	−0.264	−0.171	2.086	5.056	0.000	0.883
N-Formylmorpholine	−0.437	0.024	2.631	4.318	0.000	0.712
N-Methylformamide	−0.249	−0.142	1.661	4.147	0.817	0.739
N-Ethylformamide	−0.220	−0.302	1.743	4.498	0.480	0.824
N-Methylacetamide	−0.197	−0.175	1.608	4.867	0.375	0.837
N-Ethylacetamide	−0.018	−0.157	1.352	4.588	0.357	0.824
Formamide	−0.800	0.310	2.292	4.130	1.933	0.442
Acetonitrile	−0.007	−0.595	2.461	2.085	0.418	0.738
Nitromethane	−0.340	−0.297	2.689	2.193	0.514	0.728
Dimethylsulfoxide	−0.556	−0.223	2.903	5.036	0.000	0.719
Sulfolane (303 K)	−0.414	0.084	2.396	3.144	0.420	0.684
Tributylphosphate	0.097	−0.098	1.103	2.411	0.588	0.844
Gas-water	−1.271	0.822	2.743	3.904	4.814	−0.213

having the same McGowan volume. The molar refraction is given by[7]

$$MR_X = 10\left[\frac{(\eta^2-1)}{(\eta^2+2)}\right]V, \tag{15}$$

where η is the refractive index of the solute as a pure liquid at 293 K, and V is in units of (cm^3 mol^{-1})/100. For compounds that are solid at 293 K, a refractive index for the liquid at 293 K can be calculated by commercial software;[39] or alternatively E can be computed by summing fragment groups in the molecule[40] or by using the PharmaAlgorithm commercial software.[41] The molar refraction is one of the few properties that is very nearly the same for a given molecule in both the gaseous and liquid state, even for associated liquid molecules such as water. The numerical value of molar refraction of the alkane molecule needed in the computation of E is given by[7]

$$(MR_X)_{\text{alkane}} = 2.83195\ V - 0.52553, \tag{16}$$

where V is the characteristic McGowan volume described above. The remaining four solute descriptors, S, A, B, and L, are calculated by solving a series of simultaneous $\log_{10} P$ and $\log_{10} K$ equations for which both experimental partition coefficient data and solvent equation coefficients (c_p, e_p, s_p, a_p, b_p, v_p, c_k, e_k, s_k, a_k, b_k, and l_k) are known. The computation method is illustrated in several published papers and will not be repeated here.

The Abraham general solvation parameter model has been used successfully to correlate the solubility behavior of several substituted benzoic acids (namely, 2-acetoxybenzoic acid, 4-aminobenzoic acid, 3-chlorobenzoic acid, 4-chlorobenzoic acid, 2-chloro-5-nitrobenzoic acid, 4-chloro-3-nitrobenzoic acid, 3,4-dichlorobenzoic acid, 3,5-dinitrobenzoic acid, 3,5-dinitro-2-methylbenzoic acid, 2-methoxybenzoic acid, 4-methoxybenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 3-nitrobenzoic acid, 4-nitrobenzoic acid) dissolved in a series of alcohols, dialkyl ethers, and alkyl alkanoates. Equations (10) and (11) described the experimental solubility data to within a standard deviation of ±0.15 $\log_{10}$ units. Past experience in using various solution models has been that the better solution will generally give predicted values that fall with ±40% or so (about ±0.15 $\log_{10}$ units) of the observed solute solubilities. The Abraham model will be used to assess the experimental solubility data for a few select substituted benzoic acids, and to identify possible values that need to be remeasured. More detailed information concerning the model will be given later in this work where actual experimental solubility is being evaluated.

The solvent composition dependence upon solubility is generally evaluated using semi-theoretical solution models. During the past 50 years, more than 100 solution models have developed for describing variation of solubility with solvent composition based on different assumptions regarding how molecules interact in solution. Predictive expressions derived from several of the proposed solution models have served as mathematical representations for isothermal solubility data in binary and ternary solvent mixtures, and for identifying experimental data points in need of redetermination. The Combined Nearly Ideal Binary Solvent (NIBS)/Redlich-Kister equation[42,43]

$$\ln x_1^{\mathrm{sat}} = x_2^{(\mathrm{s})} \ln(x_1^{\mathrm{sat}})_2 + x_3^{(\mathrm{s})} \ln(x_1^{\mathrm{sat}})_3 + x_2^{(\mathrm{s})} x_3^{(\mathrm{s})} \sum_{j=0}^{r} S_{23,j}(x_2^{(\mathrm{s})} - x_3^{(\mathrm{s})})^j \qquad (17)$$

is likely the most popular of the proposed mathematical representations. In the above equation, $x_i^{(\mathrm{s})}$ refers to the initial mole fraction solvent composition of component i calculated as if the solute were not present, and $(x_{\mathrm{A}}^{\mathrm{sat}})_i$ denotes the measured solute solubility in pure solvent i. The summation in the last term on the right-hand side of Eq. (17) includes as many curve-fit $S_{23,j}$ parameters as are needed to accurately describe the observed solubility data. Generally no more than three parameters will be needed in a given mathematical representation. The various $S_{23,j}$ parameters are determined by regression analysis.

The popularity of the Combined NIBS/Redlich-Kister model results from the fact that the computed $S_{IJ,i}$ parameters can be used to predict solute solubility in ternary solvent systems:

$$\begin{aligned}\ln x_1^{\mathrm{sat}} = {} & x_2^{(\mathrm{s})}\ln(x_1^{\mathrm{sat}})_2 + x_3^{(\mathrm{s})}\ln(x_1^{\mathrm{sat}})_3 + x_4^{(\mathrm{s})}\ln(x_1^{\mathrm{sat}})_4 \\ & + x_2^{(\mathrm{s})} x_3^{(\mathrm{s})} \sum_{j=0}^{r} S_{23,j}(x_2^{(\mathrm{s})} - x_3^{(\mathrm{s})})^j \\ & + x_2^{(\mathrm{s})} x_4^{(\mathrm{s})} \sum_{k=0}^{s} S_{24,k}(x_2^{(\mathrm{s})} - x_4^{(\mathrm{s})})^k \\ & + x_3^{(\mathrm{s})} x_4^{(\mathrm{s})} \sum_{l=0}^{t} S_{34,l}\,(x_3^{(\mathrm{s})} - x_4^{(\mathrm{s})})^l \end{aligned} \qquad (18)$$

and in higher-order multicomponent solvent systems:

$$\ln x_1^{\mathrm{sat}} = \sum_{I}^{\mathrm{Solvents}} \sum_{J>I}^{\mathrm{Solvents}} \left[x_I^{(\mathrm{s})} x_J^{(\mathrm{s})} \sum_{k=0}^{n} S_{IJ,k}(x_I^{(\mathrm{s})} - x_J^{(\mathrm{s})})^k \right]. \qquad (19)$$

Equation (18) is referred to as the Combined Nearly Ideal Ternary Solvent (NITS)/Redlich-Kister model. To date Eq. (18) has been shown to provide very accurate predictions for the solubility of anthracene and/or pyrene in 114 different ternary solvent mixtures including several alcohol + hydrocarbon + hydrocarbon, alcohol + alcohol + hydrocarbon, alkoxyalcohol + alcohol + hydrocarbon, alkoxyalcohol + alcohol + alcohol, and alkyl ether + alcohol + hydrocarbon solvent systems.[44–46]

2. Solubility of Benzoic Acid in Organic Solvents

2.1. Critical evaluation of experimental solubility data

There have been numerous studies[47–91] involving the solubility of benzoic acid in organic solvents, particularly at 298 K. Most notably, Beerbower *et al.*[47] measured the solubility in 57 different organic solvents, including six saturated hydrocarbons (pentane, hexane, heptane, nonane, decane, and cyclohexane), two aromatic hydrocarbons (benzene and methylbenzene), one dialkyl ether (1,1′-oxybisethane) and one cyclic ether (1,4-dioxane), two alkyl alkanoates (ethyl ethanoate and butyl ethanoate), three chloroalkanes (trichloromethane, tetrachloromethane, and 1,2-dichloroethane) and one chlorinated aromatic hydrocarbon (chlorobenzene), 12 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-methyl-1-propanol, 1-pentanol, 1-hexanol, 1-octanol, 1,2-ethanediol, 1,2,3-propanetriol, and benzenemethanol), one alkanone (propanone) and one aromatic ketone (acetophenone), and nine miscellaneous organic solvents (nitrobenzene, ethanoic acid, propanoic acid, dimethyl sulfoxide, pyridine, formamide, *N*-methylformamide, *N*,*N*-dimethylformamide, and *N*,*N*-dimethylacetamide). The experimental data were used to test the limitations and applications of the Expanded Solubility Parameter Approach. Restaino and Martin[75] published solubility data for benzoic acid in 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, and 1-octanol. Acree and Bertrand,[49] Perlovich and Bauer-Brandl,[53] Gomaa,[64] Ongley,[56] Thuaire,[72] Yurquina *et al.*,[78] and Chantooni and Kolthoff[76] have also performed benzoic acid solubility measurements at 298 K.

The Abraham solvation parameter model can provide an indication of the quality of experimental solubility data for benzoic acid dissolved in a series of organic solvents of varying polarity and hydrogen bonding character. As discussed above, the evaluation will be restricted to those solvents where dimerization is not likely to occur and to solvents where benzoic acid does not form a solid solvate. Expressions based on the Abraham model have been shown to provide reasonably accurate mathematical correlations for the solubility behavior of numerous crystalline nonelectrolyte solutes, with deviations between observed and calculated values on the order of

0.15 $\log_{10}$ units or less. Several of the published studies have involved substituted benzoic acids. Results of these studies will be discussed later in the volume as the solubility data of the respective solutes are presented.

The Abraham model is based on two linear free energy relationships that describe solute transfer to organic solvents from water and from the gas phase. Expressed in terms of molar solubility, the linear free energy relationships take the following mathematical forms

$$\log_{10}(c_{1,\mathrm{S}}^{\mathrm{sat}}/c_{1,\mathrm{W}}^{\mathrm{sat}}) = c_{\mathrm{p}} + e_{\mathrm{p}} \cdot E + s_{\mathrm{p}} \cdot S + a_{\mathrm{p}} \cdot A + b_{\mathrm{p}} \cdot B + v_{\mathrm{p}} \cdot V, \tag{20}$$

$$\log_{10}(c_{1,\mathrm{S}}^{\mathrm{sat}}/c_{1,\mathrm{G}}) = c_{\mathrm{k}} + e_{\mathrm{k}} \cdot E + s_{\mathrm{k}} \cdot S + a_{\mathrm{k}} \cdot A + b_{\mathrm{k}} \cdot B + l_{\mathrm{k}} \cdot L, \tag{21}$$

where $c_{1,\mathrm{S}}^{\mathrm{sat}}$ and $c_{1,\mathrm{W}}^{\mathrm{sat}}$ are the molar solubilities of the solute in the organic solvent and in water, respectively, and $c_{1,\mathrm{G}}$ is the molar concentration of the solute in the gas phase. The molar concentrations are expressed in units of mol dm^{-3}. For notational simplicity the "sat" superscript will be dropped in subsequent discussions, and the quantities simply denoted as c_1 and $c_{1,\mathrm{W}}$. The Abraham model solvent equation coefficients that are given in Tables 1 and 2 pertain to 298 K unless otherwise noted. For a given solute-solvent system, Eqs. (20) and (21) give calculated c_1 values that differ from one another by only a few hundredths of a $\log_{10}$ unit.

Numerical values of the solute descriptors for benzoic acid are known ($E = 0.730$, $S = 0.900$, $A = 0.590$, $B = 0.400$, and $V = 0.9317$), so that combination of these descriptors with the coefficients listed in Table 1 permit the prediction of $\log_{10}(c_{1,\mathrm{S}}^{\mathrm{sat}}/c_{1,\mathrm{W}}^{\mathrm{sat}})$. The molar solubility of molecular benzoic acid in water, $\log_{10} c_{1,\mathrm{W}}^{\mathrm{sat}} = -1.55$, is available to convert the predicted $(c_{1,\mathrm{S}}^{\mathrm{sat}}/c_{1,\mathrm{W}}^{\mathrm{sat}})$ solubility ratios to $c_{1,\mathrm{S}}^{\mathrm{sat}}$ values. For carboxylic acid solutes, $c_{1,\mathrm{W}}^{\mathrm{sat}}$ corresponds to the aqueous solubility of the molecular, nonionized form of the solute.

The predicted molar solubilities of benzoic acid in methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, 1-octanol, 1-decanol, 2-propanol, 2-butanol, 2-pentanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 3-methyl-1-butanol, 1,2-ethanediol, 1,1′-oxybisethane, 2-methoxy-2-methylpropane, tetrahydrofuran, 1,4-dioxane, methyl ethanoate, ethyl ethanoate, propyl ethanoate, butyl ethanoate, and propanone based on Eq. (20) are listed in the second column of Table 3. Alkane and aromatic hydrocarbon solvents are excluded from consideration because of dimerization concerns. The numerical values represent outright solubility predictions in that none of the experimental data was used in the determination of the molecular solute descriptors. For comparison purposes, the measured mole fraction solubilities of benzoic acid, x_1, given

TABLE 3. Comparison between observed and predicted molar solubilities of benzoic acid based on the Abraham model, Eq. (20)

Solvent	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{exp}}$
Methanol	0.449	0.504[a]		0.228[b]	
Ethanol	0.432	0.427[a]		0.292[b]	0.441[c]
1-Propanol	0.311	0.348[a]	0.366[d]		
2-Propanol	0.322	0.372[a]			
1-Butanol	0.215	0.329[a]	0.332[d]		
2-Butanol	0.257				
2-Methyl-1-propanol	0.178	0.209[a]			
2-Methyl-2-propanol	0.323	0.398[e]			
1-Pentanol	0.221	0.232[a]	0.322[d]		
2-Pentanol	0.237				
3-Methyl-1-butanol	0.166				
1-Hexanol	0.166	0.196[a]	0.220[d]		
1-Heptanol	0.105	0.160[f]			
1-Octanol	0.055	0.129[a]	−0.070[d]		
1-Decanol	−0.005				
1,2-Ethanediol	0.068	0.167[a]	0.176[h]		
1,1′-Oxybisethane	0.047	0.243[a]			
2-Methoxy-2-methylpropane	−0.001				
Tetrahydrofuran	0.625				
1,4-Dioxane	0.359	0.496[a]		0.371[b]	
Methyl ethanoate	0.108				
Ethyl ethanoate	0.138	0.220[a]			
Propyl ethanoate	0.067				
Butyl ethanoate	−0.005	0.124[a]			
Propanone	0.295	0.368[a]	0.382[g]		

[a] Experimental value is taken from Beerbower *et al.*[47]
[b] Experimental value is taken from Gomaa.[64]
[c] Experimental value is taken from Thuaire.[72]
[d] Experimental value is taken from Restaino and Martin.[75]
[e] Experimental value is from Chantooni and Kolthoff.[76]
[f] Experimental value is from Perlovich and Bauer-Brandl.[53]
[g] Experimental value is from Long *et al.*[55]
[h] Experimental value is from Yurquina *et al.*[78]

TABLE 4. Recommended mole fraction solubilities for benzoic acid in select solvents

Solvent	Recommended value	Individual values	Outliers
Cyclohexane	0.0107	0.0102,[47] 0.01095,[55] 0.0100,[56] 0.0115 (Ref. 49)	
Benzene	0.0731	0.073,[59] 0.0728,[58] 0.0734 (Ref. 47)	
Methylbenzene	0.0728	0.0734,[47] 0.071,[48] 0.0741 (Ref. 58)	
Tetrachloromethane	0.0495	0.0494,[47] 0.0500,[67] 0.0492 (Ref. 49)	
Methanol	0.163	0.1632,[47] 0.1569,[51] 0.1693 (Ref. 68)	0.0771 (Ref. 64)
Ethanol	0.183	0.1789,[47] 0.1808,[71] 0.1855,[72] 0.1882 (Ref. 50)	0.1264 (Ref. 64)
1-Propanol	0.180	0.1791,[47] 0.1743,[51] 0.187,[75] 0.1810 (Ref. 50)	
Propanone	0.196	0.1857,[47] 0.1925,[55] 0.209 (Ref. 79)	
Ethanoic acid	0.156	0.1675,[47] 0.148,[55] 0.151 (Ref. 80)	0.1097 (Ref. 79)
N,*N*-Dimethylformamide	0.478	0.4909,[47] 0.4724,[80] 0.470 (Ref. 82)	0.2228 (Ref. 64)

in Secs. 2.2–2.10 were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\text{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\text{solvent}}]$). The molar volume of the hypothetical subcooled liquid benzoic acid is taken to be $V_{\text{solute}} = 104.38\ \text{cm}^3\ \text{mol}^{-1}$. Any errors resulting from the estimation of benzoic acid's hypothetical subcooled liquid molar volume, V_{solute}, or the ideal molar volume approximation will have negligible effect of the calculated c_1 values because benzoic acid is not overly soluble in many of the solvents considered. From a mathematical standpoint, the $x_1^{\text{exp}}V_{\text{solute}}$ term contributes very little to the molar volumes of the saturated solutions.

Examination of the numerical entries in Table 3 reveals that expressions based on the Abraham model provide a very reasonable estimate of the solubility behavior of benzoic acid in 1,1′-oxybisethane, 1,4-dioxane, propanone and in 12 alcohol and two alkyl ethanoate solvents. Standard deviations between predicted and observed values were on the order of 0.12 $\log_{10}$ units or less for most solvents. Differences in chemical purities and experimental methodologies can account for differences of several percent between values determined by different research groups.

Solution models, such as the Abraham solvation parameter model, prove useful in screening datasets for obvious outliers, particularly in cases where there are only one or two experimental data points for a given solute-solvent system. Readers are reminded that such models are only able to identify those outliers that fall outside of the model's expected predictive applicability. There is a sufficient number of data points for several of the solvents in Secs. 2.2–2.11 to compute a recommended value. The criterion that is used here to give a recommended value is that there must be at least three independent solubility measurements that differ from each other by no more than approximately 15 relative percent. Moreover, there must not be too many data points that fall outside of this range. The recommended mole fraction solubilities were calculated as an arithmetic average and are given in Table 4 for the solvents that had three or more close solubility measurements. Included in the table are the individual mole fraction solubilities that went into the calculation, and any suspected outlier values. There are a couple of instances were two independent experimental values are close and a third value differs by more than 30 relative percent. For example, in the case of ethyl ethanoate there are two close values $x_1 = 0.1649$ (Ref. 47) and $x_1 = 0.1637$ (Ref. 31) which differ significantly from a third value of $x_1 = 0.229$,[57] in the case of trichloromethane there are two close values of $x_1 = 0.1283$ (Ref. 47) and $x_1 = 0.132$ (Ref. 48) which differ significantly from a third value of $x_1 = 0.273$,[57] and in the case of 1-octanol there are two close values of $x_1 = 0.1987$ (Ref. 47) and $x_1 = 0.185$ (Ref. 77) which differ significantly from a third value of $x_1 = 0.129$.[75] The latter value in each of the three listings is believed to be an outlier.

There have been several experimental studies examining the solubility of benzoic acid in different organic solvents as a function of temperature. Thati *et al.*[48] determined benzoic acid solubilities in pentane, heptane, cyclohexane, methylbenzene, ethanol, and trichloromethane, and in binary heptane + ethanol and methylbenzene + ethanol solvent mixtures, in the approximate temperature range from 278 to 323 K. The authors described the variation of ln x_1 with temperature in terms of

$$\ln x_1 = A + \frac{B}{T} + C\,T, \tag{22}$$

a relatively simple nonlinear equation. The calculated regression coefficients (A, B, and C) are listed in Table 5, along with the actual temperature range for each of the six monosolvents. The authors noted that the squared correlation coefficient, R^2, exceeded 0.9996. The graphical comparison provided in the paper indicated very good agreement between the experimental x_1 data and back-calculated values based on Eq. (22).

Zhao *et al.*[60] measured the solubility of benzoic acid in isobutyl ethanoate at 18 temperatures between 300 and 343 K. The experimental data were correlated with the Wilson and UNIQUAC models. Interaction coefficients calculated from the experimental solid-liquid equilibrium data provided a reasonably accurate mathematical description of the measured values. The mean absolute relative deviation between calculated and observed values was 0.85% (Wilson model) and 1.06% (UNIQUAC model).

TABLE 5. Parameters of Eq. (22) for describing the solubility of benzoic acid in various organic solvents[a]

Solvent	T/K	A	B	C
Pentane	278–303	−20.9245	444.93	0.04932
Heptane	278–323	−8.4537	−3803.41	−0.00032
Cyclohexane	283–323	−7.9394	−1683.88	0.03071
Methylbenzene	278–323	−0.4993	−1927.02	0.01466
Trichloromethane	278–323	−0.2008	−1492.75	0.01066
Ethanol	278–323	−6.1372	−102.31	0.01599

[a] Values of the coefficients were taken from Thati *et al.*[48]

TABLE 6. Parameters of the Van't Hoff-type equation for describing the solubility of benzoic acid in various organic solvents

Solvent	T/K	A	B	C	MRD (%)
Cyclohexane[a]	283–343	−8.5248	8766.1	2 259 000	2.75
2-Propanol[a]	278–343	3.9085	−11624.0	−9250	0.54
Propanone[a]	278–323	6.0996	−2925.6	184 060	0.63
Ethanoic acid[a]	293–346	4.8518	−1721.8	−88 300	0.62

[a] Values of the coefficients and mean relative deviation were taken from Long *et al.*[55]

Long *et al.*[55] published experimental solubility data for benzoic acid in cyclohexane, 2-propanol, propanone, and ethanoic acid over the approximate temperature range between 277 and 346 K at 5 K intervals using a gravimetric method. Experimental measurements showed that the benzoic acid solubility was greatest in propanone, followed by 2-propanol, ethanoic acid, and cyclohexane in descending order. The authors correlated the temperature dependence with a Van't Hoff-type relation:

$$\ln x_1 = A + \frac{B}{T} + \frac{C}{T^2}, \tag{23}$$

where A, B, and C represent the empirical curve-fit parameters determined by regression analysis of $\ln x_1$ data in accordance with Eq. (23). The calculated equation coefficients and the mean relative deviation (MRD) defined by Eq. (24) below

$$\mathrm{MRD}\,(\%) = \frac{100}{N} \sum \left| \frac{(x_1{}^{\mathrm{exp}} - x_1{}^{\mathrm{calc}})}{x_1{}^{\mathrm{exp}}} \right| \tag{24}$$

are tabulated in Table 6. In Eq. (24), N denotes the number of experimental solubility measurements in an individual solute-solvent dataset. Examination of the numerical values in the last column of Table 6 indicates that Eq. (23) does provide a reasonably accurate mathematical description of how the solubility varies with temperature. The small mean relative deviations suggest that the experimental values in each solvent dataset are internally consistent.

Ma and Xia[80] determined the solubility of benzoic acid in both ethanoic acid and *N*,*N*-dimethylformamide. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to the Buchowski λh model [Eq. (9)]. The values of the equation coefficients (λ and h) are given in Table 7, along with the mean relative deviation. Also included in Table 7 are the equation coefficients reported by Cheng *et al.*[90] for the solubility of benzoic acid in ethanol, benzene, ethanoic acid, and ethyl ethanoate. The authors performed solubility measurements over the temperature range of 291–356 K and reported their results only in the form of curve-fit equation coefficients. The actual mole fraction solubility data was not given in the published paper. The small mean relative deviations suggest that the experimental values in each solvent dataset are internally consistent. Readers are reminded that Eq. (9) can only check data points for internal consistency with respect to temperature. The fact that one can accurately describe the experimental data does not mean that the data are accurate. In the case of ethanoic acid, there are three sets of independent solubility data in the published literature. A point-by-point comparison will not be performed here; however, one does note that the experimental solubilities reported by Long *et al.*[55] and Ma and Xia[80] are in reasonably good agreement with each other at 298 K [$x_1 = 0.1481$ (Ref. 55) versus $x_1 = 0.1448$ (Ref. 80)] and 318 K [$x_1 = 0.2367$ (Ref. 55) and $x_1 = 0.2384$ (Ref. 80)], and both sets of values differ from those reported by Wang *et al.*,[79] which are $x_1 = 0.1097$ at 298 K and $x_1 = 0.1576$ at 318 K.

TABLE 7. Parameters of the Buchowski λh equation for describing the solubility of benzoic acid in various organic solvents

Solvent	T/K	λ	h	MRD (%)
Ethanoic acid[a]	291–334	0.7767	2614.61	0.67
Ethanoic acid[b]	291–356	0.8061	2594.9	0.58
N,*N*-Dimethylformamide[a]	299–343	−0.6448	2379.67	0.13
Benzene[b]	291–356	1.5203	2438.3	0.36
Ethyl ethanoate[b]	291–356	0.6058	2656.9	0.31
Ethanol[b]	291–356	0.3918	3212.2	0.28

[a] Values of the coefficients and mean relative deviation were taken from Ma and Xia.[80]

[b] Values of the coefficients and mean relative deviation were taken from Cheng *et al.*[90]

Li *et al.*[84] determined the solubility of benzoic acid in *N*-methyl-2-pyrrolidone from 296 to 371 K using a synthetic method with laser monitoring to determine when the last amount of solid solute dissolved. The authors employed a polynomial expression in temperature,

$$x_1 = -6.0581 + 0.06480\,T - 2.17813 \times 10^{-4}\,T + 2.49784 \times 10^{-7} T^2, \tag{25}$$

to represent the measured mole fraction solubility data. The root-mean-square deviation between the observed x_1 and calculated values from Eq. (25) was on the order of 0.0012 mole fraction.

The experimental solubility data for benzoic acid in organic solvents are in Secs. 2.2–2.11.

2.2. Benzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components: (1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Pentane; C_5H_{12}; [109-66-0]	**Original Measurements:** [47] A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9941	0.0059

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Pentane; C_5H_{12}; [109-66-0]	[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.996	0.004
283.15	0.995	0.005
293.15	0.991	0.009
303.15	0.989	0.011

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 95+%, VWR Scientific, USA, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Hexane; C_6H_{14}; [110-54-3]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9905	0.0095

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Hexane; C_6H_{14}; [110-54-3]	[49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.15	0.9900	0.0100
303.15	0.9874	0.0126

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99%, Chemical source not given, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Hexane; C_6H_{14}; [110-54-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9860	0.01399

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Hexane; C_6H_{14}; [110-54-3]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9870	0.0130

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Hexane; C_6H_{14}; [110-54-3]	[52]A. Ksiazczak, Fluid Phase Equilib. **28**, 57 (1986).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
312.55	0.9812	0.0188
316.30	0.9773	0.0227
319.57	0.9737	0.0263
319.85	0.9734	0.0264
321.48	0.9711	0.0289
321.52	0.9709	0.0291
322.85	0.9698	0.0302
323.48	0.9685	0.0315
325.50	0.9660	0.0340
325.80	0.9652	0.0348
327.49	0.9630	0.0370
327.50	0.9630	0.0370
329.47	0.9595	0.0405

T/K	x_2[a]	x_1[b]
331.45	0.9564	0.0436
333.48	0.9530	0.0470
333.50	0.9525	0.0475
335.48	0.9476	0.0524
336.10	0.9454	0.0546
336.15	0.9445	0.0555
338.47	0.9395	0.0605
339.50	0.9363	0.0637
341.55	0.9299	0.0701
341.65	0.9291	0.0709
343.52	0.9230	0.0770
344.50	0.9198	0.0802
344.60	0.9186	0.0814
345.48	0.9152	0.0848
347.40	0.9065	0.0935
347.46	0.9067	0.0933
349.30	0.899	0.101
350.30	0.893	0.107
351.41	0.888	0.112
353.50	0.876	0.124
356.45	0.855	0.145
359.40	0.832	0.168
362.60	0.798	0.202

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined using a dynamic method. Known amounts of solute and solvent were placed in a container which was then sealed. The temperature of the solution was slowly increased until the last amount of solid dissolved. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, POCh Gliwice, Poland, was dried over phosphorous pentoxide and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Heptane; C_7H_{16}; [142-82-5]	[47] A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9883	0.0117

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Heptane; C_7H_{16}; [142-82-5]	[48] J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.995	0.005
283.15	0.994	0.006
293.15	0.990	0.010
303.15	0.985	0.015
313.15	0.978	0.022
323.15	0.967	0.033

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 99%, VWR Scientific, USA, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Heptane; C_7H_{16}; [142-82-5]	[49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.15	0.9886	0.0114
303.15	0.9853	0.0147

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99+%, Chemical source not given, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Octane; C_8H_{18}; [111-65-9]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9871	0.0129

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and analytical balance. Very little experimental details were given in the paper. The solubility of the solute was by a weighing method.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Sigma Chemical Company, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±3.0% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Nonane; C_9H_{20}; [111-84-2]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9859	0.0141

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9898	0.0102

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9898	0.0102

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9857	0.0143

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[55]B. Long, J. Li, R. Zhang, and L. Wan, Fluid Phase Equilib. **297**, 113 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.9968	0.003179
287.95	0.9953	0.004724
293.16	0.9926	0.007413
298.00	0.9890	0.01095
303.30	0.9847	0.01528
308.02	0.9795	0.02052
313.18	0.9698	0.03023
317.75	0.9630	0.03701
322.91	0.9532	0.04678
328.18	0.9434	0.05656
333.11	0.9275	0.07254
337.98	0.9066	0.09341
342.80	0.8777	0.1223

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Double layer jacketed glass equilibrium cell, circulating water bath, analytical balance, and drying oven.
Excess solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was allowed to equilibrate at constant temperature with stirring for 3 h. The stirring was discontinued and the solution was allowed to stand for 1 h to allow the undissolved solid to settle to the bottom portion of the equilibrium vessel. An aliquot of the clear solution was transferred to a preweighed vial by a warm syringe. The vial was tightly closed and reweighed to determine the mass of the sample transferred. The vial was then put into a drying oven with the cap half-closed to permit complete evaporation of the solvent. The vial was covered with a piece of stainless steel filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was removed from the drying oven and placed in a desiccator with silica gel for another 2 h to reach ambient room temperature. The vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Analytical grade, Shantou Xilong Chemical Company, China, was used as received.
(2) 99.5%, Analytical grade, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[52]A. Ksiazczak, Fluid Phase Equilib. **28**, 57 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
309.65	0.9802	0.0198
315.45	0.9745	0.0255
318.20	0.9700	0.0300
320.95	0.9654	0.0346
325.35	0.9564	0.0436
329.00	0.9494	0.0506
332.60	0.9366	0.0634
334.45	0.9302	0.0698
338.80	0.9118	0.0882
339.00	0.9110	0.0890
341.35	0.9005	0.0995
342.95	0.890	0.110
343.55	0.888	0.112
345.55	0.873	0.127
346.55	0.867	0.133
347.30	0.863	0.137
349.35	0.846	0.154
349.50	0.841	0.159
351.15	0.830	0.170
351.55	0.823	0.177
354.50	0.786	0.214
360.65	0.695	0.305
366.35	0.574	0.426
369.40	0.514	0.486
372.35	0.448	0.552
375.50	0.391	0.609
379.40	0.305	0.695
383.80	0.235	0.765
389.85	0.115	0.885

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined using a dynamic method. Known amounts of solute and solvent were placed in a container which was then sealed. The temperature of the solution was slowly increased until the last amount of solid dissolved. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, POCh Gliwice, Poland, was dried over phosphorous pentoxide and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.15	0.9885	0.0115
303.15	0.9854	0.0146

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99+%, Chemical source not given, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.15	0.994	0.006
293.15	0.991	0.009
303.15	0.985	0.015
313.15	0.975	0.025
323.15	0.961	0.039

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 99.5%, VWR Scientific, USA, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.038$, which corresponds to a solubility of $c_1 = 0.0916$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

2.3. Benzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9311	0.0689

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9168	0.0832

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.118$, which corresponds to a solubility of $c_1 = 0.762\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1916).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.931	0.069

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance and a steam bath.
Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9181	0.08191

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2]	[58]J. Chipman, J. Am. Chem. Soc. **46**, 2445 (1924).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values (Interpolated Values)

T/K	x_2[a]	x_1[b]
277.5	0.967	0.0332
283.2	0.966	0.0339
293.2	0.941	0.0594
298.2	0.927	0.0728
303.2	0.912	0.0879
313.2	0.874	0.1261
323.2	0.821	0.1794
333.2	0.751	0.249
343.2	0.663	0.337
353.2	0.556	0.444
363.2	0.432	0.568
373.2	0.302	0.698
383.2	0.165	0.835

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solid-liquid equilibrium temperatures and mole fraction compositions represent interpolated values obtained from the actual experimental data. The actual experimental data were not given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Water bath, glycerol bath, and stirrer.
Solubilities were determined in a 2.5 × 15 cm air-jacketed test-tubes using short-stemmed thermometers. The tube, together with the thermometer, cork stopper, and stirrer were weighed, benzoic acid was then added, and the entire assembly reweighed again. The total weight of the mixture was determined again after the solid-liquid equilibrium temperature had been recorded in order to avoid errors due to solvent evaporation. The mixture of benzoic acid and solvent was heated in a water bath or glycerol bath until entirely homogeneous. The mixture cooled with rapid stirring to form a suspension of minute crystals, and then warmed slowly (about 0.5 K/ min) with continuous stirring until all of the crystals dissolved. The temperature at which the solution became clear was recorded as the solid-liquid equilibrium temperature.
The experimental solubilities at the three lower temperatures were determined by titration. Glass-stoppered bottles containing excess solute and solvent were allowed to equilibrate at constant temperature in a thermostat. An aliquot of the clear saturated solution was removed and transferred into a glass-stoppered Erlenmeyer flask and weighed. A measured amount of slight excess sodium hydroxide solution was added, and the excess sodium hydroxide was determined by back titration with a standardized acetic acid solution with phenolphthalein being used to detect the endpoint. The solvent was evaporated in a current of carbon dioxide-free air.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized successively from 50% aqueous-acetic acid solution, benzene, three times from 30% aqueous-alcohol, and twice from pure benzene. The melting point of the purified sample was 394.9 K.
(2) Purity not given, Chemical source not given, was shaken repeatedly with sulfuric acid, and then successively with water, dilute aqueous sodium hydroxide solution, water, and saturated calcium chloride solution. The sample was then fractionally distilled over solid calcium chloride, then frozen out and finally distilled from metallic sodium.

Estimated Error:
Temperature: Unable to determine.
x_1: Unable to determine.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2]	[59]H. Buchowski, J. Solution Chem. **20**, 139 (1991).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values (Interpolated Values)

T/K	x_2[a]	x_1[b]
298.15	0.927	0.073
300.15	0.921	0.079
302.15	0.915	0.085
313.15	0.874	0.126
318.15	0.850	0.150
323.15	0.821	0.179
328.15	0.790	0.210
333.15	0.751	0.249

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided in the paper. In the author's earlier studies, solubilities were determined using a dynamic solubility method where known amounts of solute and solvent were placed in containers which were then sealed. The temperature was then slowly increased until all of the solid solute dissolved. The compiler believes that the benzoic acid solubilities in the present study may have been determined by a similar method. The tabulated numerical values might be interpolated values obtained from a smooth mole fraction versus temperature curve.

Source and Purity of Chemicals:
(1) 99.5%, Argon, Lodz, Poland, purified by at least two vacuum sublimations.
(2) 99.5%, POCh, Gliwice, Poland, was dried over phosphorous pentoxide and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methylbenzene; C_7H_8; [108-88-3]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9266	0.0734

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methylbenzene; C_7H_8; [108-88-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9145	0.08553

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methylbenzene; C_7H_8; [108-88-3]	[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.965	0.035
283.15	0.957	0.043
293.15	0.938	0.062
303.15	0.911	0.089
313.15	0.872	0.128
323.15	0.822	0.178

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 99+%, Merck Chemical Company, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methylbenzene; C_7H_8; [108-88-3]	[58]J. Chipman, J. Am. Chem. Soc. **46**, 2445 (1924).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values (Interpolated Values)

T/K	x_2[a]	x_1[b]
273.2	0.964	0.0339
283.2	0.958	0.0423
293.2	0.938	0.0618
298.2	0.926	0.0741
303.2	0.911	0.0891
313.2	0.873	0.1270
323.2	0.821	0.1790
333.2	0.753	0.247
343.2	0.667	0.333
353.2	0.561	0.439
363.2	0.439	0.561
373.2	0.304	0.696
383.2	0.166	0.834

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solid-liquid equilibrium temperatures and mole fraction compositions represent interpolated values obtained from the actual experimental data. The actual experimental data were not given in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
Water bath, glycerol bath, and stirrer.
Solubilities were determined in a 2.5 × 15 cm air-jacketed test-tubes using short-stemmed thermometers. The tube, together with the thermometer, cork stopper, and stirrer were weighed, benzoic acid was then added, and the entire assembly reweighed again. The total weight of the mixture was determined again after the solid-liquid equilibrium temperature had been recorded in order to avoid errors due to solvent evaporation. The mixture of benzoic acid and solvent was heated in a water bath or glycerol bath until entirely homogeneous. The mixture cooled with rapid stirring to form a suspension of minute crystals, and then warmed slowly (about 0.5 K/min) with continuous stirring until all of the crystals dissolved. The temperature at which the solution became clear was recorded as the solid-liquid equilibrium temperature.
The experimental solubilities at the three lower temperatures were determined by titration. Glass-stoppered bottles containing excess solute and solvent were allowed to equilibrate at constant temperature in a thermostat. An aliquot of the clear saturated solution was removed and transferred into a glass-stoppered Erlenmeyer flask and weighed. A measured amount of slight excess sodium hydroxide solution was added, and the excess sodium hydroxide was determined by back titration with a standardized acetic acid solution with phenolphthalein being used to detect the endpoint. The solvent was evaporated in a current of carbon dioxide-free air.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized successively from 50% aqueous-acetic acid solution, benzene, three times from 30% aqueous-alcohol, and twice from pure benzene. The melting point of the purified sample was 394.9 K.
(2) Purity not given, Chemical source not given, was shaken repeatedly with sulfuric acid, and then successively with water, dilute aqueous sodium hydroxide solution, water, and saturated calcium chloride solution. The sample was then fractionally distilled over solid calcium chloride, and then distilled from metallic sodium.

Estimated Error:
Temperature: Unable to determine.
x_1: Unable to determine.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9111	0.0889

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

2.4. Benzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8351	0.1649

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8363	0.1637

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1916).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.771	0.229

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath.
Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[89]S. J. Lloyd, J. Phys. Chem. **22**, 300 (1918).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
266.7	0.0655
294.7	0.309
348.2	0.784

[a]c_1: molar solubility of the solute expressed in units of mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details were not provided in the paper. Solubility measurements were performed as part of a study of the electrolytic decomposition of benzoic acid in ethyl ethanoate.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification details were not provided.
(2) Purity not given, Chemical source not given, purification details were not provided.

Estimated Error:
Temperature: Insufficient information to estimate.
c_1: Insufficient information to estimate.

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8301	0.1699

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 197.80 mg/ml, which corresponds to a molar solubility of $c_1 = 1.620\ \mathrm{mol\ dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Aldrich Chemical Company, UK, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.27.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Isobutyl ethanoate; $C_6H_{12}O_2$; [110-19-0]	[60]S. Zhao, X. Chen, Q. Dai, and L. Wang, J. Chem. Eng. Data **56**, 2399 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
299.73	0.860	0.140
302.46	0.851	0.149
307.34	0.822	0.178
313.61	0.792	0.208
322.93	0.746	0.254
328.98	0.707	0.293
332.24	0.689	0.311
334.34	0.675	0.325
335.58	0.663	0.337
336.03	0.662	0.338
337.33	0.651	0.349
337.67	0.649	0.351
338.76	0.642	0.358
339.37	0.638	0.362
339.86	0.631	0.369
341.48	0.621	0.379
342.69	0.610	0.390
343.67	0.601	0.399

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermoelectric circulating water temperature controller, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate 1-2 K/h (0.5–1.0 K/h or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.
(2) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.001.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Methylethyl tetradecanoate; $C_{17}H_{34}O_2$; [110-27-0]	[61]E. R. Cooper, J. Controlled Release **1**, 153 (1984).
Variables:	**Prepared by:**
T/K = 295	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.896	0.104

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Matheson, Coleman, and Bell, Cincinnati, OH, USA, no purification details provided.
(2) Reagent grade, Wickhen Corporation, Huguenot, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Methylethyl tetradecanoate; $C_{17}H_{34}O_2$; [110-27-0]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 41.30 mg/ml, which corresponds to a molar solubility of $c_1 = 0.338$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Croda Universal Ltd., no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.0066.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2,3-Triacetoxypropane; $C_9H_{14}O_6$; [102-76-1]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8588	0.1412

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Purity not given, Unichema International, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

2.5. Benzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8163	0.1837

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1916).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.917	0.083

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath.
Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Dimethoxyethane; $C_4H_{10}O_2$; [110-71-4]	[62]S. H. Ghosh and D. K. Hazra, J. Chem. Soc., Perkin Trans. 2 **1989**, 1021.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $c_1 = 3.2025$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Mechanical shaker and a constant-temperature thermostat.
Excess solute and solvent were placed in a Campbell solubility apparatus and allowed to equilibrate at 298 K for 24 h. An aliquot of the saturated solution was then removed and filtered. The concentration of the dissolved solute was determined by titration with standard caustic soda using phenolphthalein as indicator. Solubility was also determined spectrophotometrically from absorbance measurements made at an analysis wavelength of 272 nm.

Source and Purity of Chemicals:
(1) G.R.E, Merck Chemical Company, was recrystallized from alcohol and then dried.
(2) Purum, Fluka, was shaken with ferrous sulfate and then distilled. The distillate was further purified by refluxing for 12 h and distilling over metallic sodium.

Estimated Error:
Temperature: ±0.01 K.
c_1: ±.5% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.620	0.380

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6652	0.3348

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7147	0.2853

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[64]E. A. Gomaa, Phys. Chem. Liq. **50**, 279 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7893	0.2107

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute, computed by the compiler. The original solubility data were given in units of moles per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature shaker bath and analytical balance.
Excess solute and solvent were placed in closed test tubes and allowed to equilibrate in a constant-temperature shaker bath for several days. The solubility was determined gravimetrically by transferring 1 ml of the saturated solution to an aluminum disk. The solvent was removed by heating with an infrared lamp. The solubility was calculated from the mass of the solid residue and amount of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.
(2) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.701	0.299

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methyl nonafluorobutyl ether; $C_5H_3F_9O$; [163702-07-6]	[65]A. F. Lagalante, A. Abdulagatov, and T. J. Bruno, J. Chem. Eng. Data **47**, 47 (2002).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values (Interpolated Values)

T/K	x_2[a]	x_1[b]
259.7	0.9999	0.000138
268.2	0.9998	0.000172
283.2	0.9997	0.000272
298.2	0.9994	0.000560
313.3	0.9989	0.00110
328.2	0.9976	0.00235

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
UV/visible spectrophotometer.
Solubilities were determined by supersaturating the solvent with naphthalene and measuring the amount of dissolved solute using a spectroscopic method. Aliquots of the saturated solution were pipetted into a volumetric flask, and diluted with acetonitrile. If necessary, the sample was further diluted to bring the measured absorbance to within the linear range of the absorbance versus calibration curve obtained from absorbance measurements on solutions of known naphthalene concentration. Absorbance measurements recorded at 272 nm.

Source and Purity of Chemicals:
(1) Purity and Chemical source were not given, was used as received.
(2) 99%, Name of commercial supplier was not given, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethyl nonafluorobutyl ether; $C_6H_5F_9O$; [163702-05-4]	[65]A. F. Lagalante, A. Abdulagatov, and T. J. Bruno, J. Chem. Eng. Data **47**, 47 (2002).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values (Interpolated)

T/K	x_2[a]	x_1[b]
259.7	0.9997	0.000282
268.2	0.9997	0.000297
283.2	0.9995	0.000459
298.2	0.9991	0.000857
313.3	0.9987	0.00133
328.2	0.9976	0.00242
343.2	0.9954	0.00463

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
UV/visible spectrophotometer.
Solubilities were determined by supersaturating the solvent with naphthalene and measuring the amount of dissolved solute using a spectroscopic method. Aliquots of the saturated solution were pipetted into a volumetric flask, and diluted with acetonitrile. If necessary, the sample was further diluted to bring the measured absorbance to within the linear range of the absorbance versus calibration curve obtained from absorbance measurements on solutions of known naphthalene concentration. Absorbance measurements recorded at 272 nm.

Source and Purity of Chemicals:
(1) Purity and Chemical source were not given, used as received.
(2) 99%, Name of commercial supplier was not given, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: 1.0% (relative error).

2.6. Benzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8717	0.1283

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.926	0.074
283.15	0.914	0.086
293.15	0.886	0.114
303.15	0.849	0.151
313.15	0.804	0.196
323.15	0.747	0.253

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 99+%, Merck Chemical Company, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = -0.188$, which corresponds to a solubility of $c_1 = 1.542$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8505	0.1495

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 1.477\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1916).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.727	0.273

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath. Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9506	0.0494

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, no information provided concerning purification.

(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	[67]M. Davies and D. M. L. Griffiths, J. Chem. Soc. **1955**, 132.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9500	0.0500

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Experimental solubility was determined by percolating the solvent at an adjustable rate through a column of solute in one limb of an U-shaped tube, a plug of cotton wool serving as support and filter. The saturated solution collects in the parallel arm and the whole is assembly is immersed in a thermostat bath except for the stoppered ends. Samples of the saturated solutions were removed and titrated with standardized carbonate-free alkali using phenolphthalein as the indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, no information provided concerning purification.

(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:

Temperature: ±0.02 K.

x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	[49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.15	0.9508	0.0492
303.15	0.9402	0.0598

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature water bath and an analytical balance.

Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:

(1) 99%, Chemical Source not given, was dried at 333 K for several h before use.

(2) 99+%, Chemical source not given, refluxed for 11 h over an aqueous solution 10% in potassium permanganate and 10% in sodium hydroxide. The tetrachloromethane was distilled off and dried with calcium hydroxide, stored in contact with mercury under an argon atmosphere, and then distilled shortly before use.

Estimated Error:

Temperature: ±0.01 K.

x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.291$, which corresponds to a solubility of $c_1 = 0.512$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: No information was given.

c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9407	0.0593

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrachloromethane; CCl_4; [56-23-5]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.549\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9305	0.0695

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,1,2,2-Tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 1.243\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,1,1,2,2-Pentachloroethane; C_2HCl_5; [76-01-7]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.893\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Dichloroethene; $C_2H_2Cl_2$; isomer was not given	[86]D. H. Wester and A. Bruins, Pharm. Weekbl. **51**, 1443 (1914).
Variables:	**Prepared by:**
T/K = 288.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9218	0.0782

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were continuously shaken in a water bath at 303 K for 1 h. The solution was then transferred to a cellar which was maintained at a constant temperature of 288 K. The solution was allowed to equilibrate in the cellar for at least two days with repeated shaking. The concentration of the dissolved solute was determined; however, the analytical method was not described.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: Not enough information in paper to estimate an uncertainty.

Components:	Original Measurements:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloroethene; C_2HCl_3; [79-06-1]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 1.116\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloroethene; C_2HCl_3; [79-06-1]	[86]D. H. Wester and A. Bruins, Pharm. Weekbl. **51**, 1443 (1914).
Variables:	**Prepared by:**
T/K = 288.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9307	0.0693

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were continuously shaken in a water bath at 303 K for 1 h. The solution was then transferred to a cellar which was maintained at a constant temperature of 288 K. The solution was allowed to equilibrate in the cellar for at least two days with repeated shaking. The concentration of the dissolved solute was determined; however, the analytical method was not described.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: Not enough information in paper to estimate an uncertainty.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Tetrachloroethene; C_2Cl_4; [127-18-4]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.660\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9138	0.0862

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8953	0.1047

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

2.7. Benzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methanol; CH_4O; [67-56-1]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8368	0.1632

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methanol; CH_4O; [67-56-1]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8431	0.1569

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methanol; CH_4O; [67-56-1]	[68]K. K. Kundu, A. L. De, and M. N. Das, J. Chem. Soc. Dalton Trans. **1972**, 386.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8307	0.1693

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details are given in paper. Authors state that a saturated solution can be obtained by mild shaking for approximately 24 h. Concentrations determined by titration with standard aqueous alkali.

Source and Purity of Chemicals:
(1) G.R. grade, Merck Chemical Company, was used as received.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methanol; CH_4O; [67-56-1]	[64]E. A. Gomaa, Phys. Chem. Liq. **50**, 279 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9229	0.0771

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute, computed by the compiler. The original solubility data were given in units of moles per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature shaker bath and analytical balance.
Excess solute and solvent were placed in closed test tubes and allowed to equilibrate in a constant-temperature shaker bath for several days. The solubility was determined gravimetrically by transferring 1 ml of the saturated solution to an aluminum disk. The solvent was removed by heating with an infrared lamp. The solubility was calculated from the mass of the solid residue and amount of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.
(2) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methanol; CH_4O; [67-56-1]	[69]C. M. McLoughlin, W. A. M. McMinn, and T. R. A. Magee, Powder Technol. **134**, 40 (2003).
Variables: T/K = 293 and 333	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 650 and 1200 g/l at 293 and 333 K, respectively. The authors did not specify whether the values were per liter of solvent or per liter of saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by adding 0.50 ± 0.1 g amounts of the powdered solute to 100 ± 1 ml of solvent until a saturated solution was obtained. The mass of the powder was recorded.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Poole, England, UK, no purification details were provided.
(2) Purity not given, Sigma-Aldrich, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
Solubility: ±5 g/l (estimated by compiler assuming solute added in increments of 0.50 g).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methanol; CH_4O; [67-56-1]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8311	0.1689

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Methanol; CH_4O; [67-56-1]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables: T/K = 308.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2223\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ± 0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[64]E. A. Gomaa, Phys. Chem. Liq. **50**, 279 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8736	0.1264

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute, computed by the compiler. The original solubility data were given in units of moles per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature shaker bath and analytical balance.
Excess solute and solvent were placed in closed test tubes and allowed to equilibrate in a constant-temperature shaker bath for several days. The solubility was determined gravimetrically by transferring 1 ml of the saturated solution to an aluminum disk. The solvent was removed by heating with an infrared lamp. The solubility was calculated from the mass of the solid residue and amount of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.
(2) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8211	0.1789

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[71]A. Seidell, Trans. Am. Electrochem. Soc. **13**, 319 (1908).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8192	0.1808

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a test tube and sealed with a rubber stopper. The test tube was attached to a rotating frame immersed in a constant-temperature water bath and revolved upon the axis parallel to the diameter of the test tube at the rate of approximately six revolutions per minute. The duration of the rotation was between four and seven days. At the end of the rotation period the test tube was placed in an upright position in the bath with the stopper and a very small part of the test tube protruding from the bath, until the undissolved solid settled to the bottom of the test tube. A portion of the clear supernatant solution was withdrawn into a pipette having a cotton plug attached. The cotton plug served as a coarse filter. The concentration of the solution was determined by titration with standard alkali solution. The author determined the solubility of benzoic acid in several aqueous-alcohol solvent mixtures having ethanol concentrations between 0.00% and 99.8% by mass. The value for 100% ethanol was obtained from the curve of solubility versus alcohol concentration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.872	0.128
283.15	0.861	0.139
293.15	0.634	0.166
303.15	0.804	0.196
313.15	0.766	0.234
323.15	0.724	0.276

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, used as received.
(2) 99+%, Solveco Chemicals, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 4.945 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1855$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[69]C. M. McLoughlin, W. A. M. McMinn, and T. R. A. Magee, Powder Technol. **134**, 40 (2003).
Variables:	**Prepared by:**
T/K = 293 and 333	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 750 and 1600 g/l at 293 and 333 K, respectively. The authors did not specify whether the values were per liter of solvent or per liter of saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by adding 0.50 ± 0.1 g amounts of the powdered solute to 100 ± 1 ml of solvent until a saturated solution was obtained. The mass of the powder was recorded.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Poole, England, UK, no purification details were provided.
(2) Purity not given, Sigma-Aldrich, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
Solubility: ±5 g/l (estimated by compiler assuming solute added in increments of 0.50 g).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 340.1 mg/ml, which corresponds to a molar solubility of $c_1 = 2.785$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, UK, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ± 0.13.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8118	0.1882

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[74]A. Pal and S. C. Lahiri, Indian J. Chem. **28A**, 276 (1989).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
288	2.2439
293	2.5042
298	2.7481

[a] c_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
A clear solution of benzoic acid, saturated at a slightly higher temperature (about 1 K higher than that of the experimental temperature) was placed in a Campbell solubility apparatus, which was then put in the experimental thermostat. The solution was allowed to equilibrate at constant temperature for approximately 4 h. An aliquot of the solution was removed and filtered. The concentration of the solute in the saturated solution was determined by titration with standardized sodium hydroxide solution.

Source and Purity of Chemicals:
(1) G.R. grade, Merck Chemical Company, Germany, was used as received.
(2) Purity not given, Chemical source not given, was purified by the standard procedure. The authors did not specify what was the standard procedure nor did was any literature method referenced.

Estimated Error:
Temperature: ±0.01 K.
c_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.872	0.128
283.15	0.861	0.139
293.15	0.834	0.166
303.15	0.804	0.196
313.15	0.766	0.234
323.15	0.724	0.276

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 99+%, Solveco Chemicals, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanol; C_2H_6O; [64-17-5]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2566\ \mathrm{mol\ dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ± 0.2 (estimated by compiler).
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8209	0.1791

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8257	0.1743

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[75]F. A. Restaino and A. N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.813	0.187

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, shaker, analytical balance, constant-temperature bath, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials and allowed to equilibrate in a constant-temperature bath with shaking for 48 h. An aliquot of the equilibrated sample was removed and filtered. Concentration of the dissolved solute was determined gravimetrically and/or spectrophotometrically. The authors did not specify which of the two methods was used for the different solutes studied.

Source and Purity of Chemicals:
(1) Certified Reagent grade, Fisher Scientific, USA, was recrsytallized from trichloromethane.
(2) Certified Reagent grade, Fisher Scientific, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8190	0.1810

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:
(1) Benzoic acid; $C_7H_6O_2$;
[65-85-0]
(2) 1-Propanol; C_3H_8O;
[71-23-8]

Original Measurements:
[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).

Variables:
T/K = 308.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2838\ \mathrm{mol\ dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical Source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:
(1) Benzoic acid; $C_7H_6O_2$;
[65-85-0]
(2) 2-Propanol; C_3H_8O;
[67-63-0]

Original Measurements:
[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8063	0.1937

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:
(1) Benzoic acid; $C_7H_6O_2$;
[65-85-0]
(2) 2-Propanol; C_3H_8O;
[67-63-0]

Original Measurements:
[55]B. Long, J. Li, R. Zhang, and L. Wan, Fluid Phase Equilib. **297**, 113 (2010).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.06	0.8714	0.1286
282.96	0.8571	0.1429
288.15	0.8405	0.1595
293.11	0.8262	0.1738
297.79	0.8078	0.1922
303.45	0.7854	0.2146
308.09	0.7679	0.2321
312.80	0.7475	0.2525
317.85	0.7220	0.2780
322.78	0.7041	0.2959
328.20	0.6749	0.3251
333.20	0.6535	0.3465
338.15	0.6265	0.3735
343.10	0.5893	0.4107

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Double layer jacketed glass equilibrium cell, circulating water bath, analytical balance, and drying oven.
Excess solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was allowed to equilibrate at constant temperature with stirring for 3 h. The stirring was discontinued and the solution was allowed to stand for 1 h to allow the undissolved solid to settle to the bottom portion of the equilibrium vessel. An aliquot of the clear solution was transferred to a preweighed vial by a warm syringe. The vial was tightly closed and reweighed to determine the mass of the sample transferred. The vial was then put into a drying oven with the cap half-closed to permit complete evaporation of the solvent. The vial was covered with a piece of stainless steel filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was removed from the drying oven and placed in a desiccator with silica gel for another 2 h to reach ambient room temperature. The vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Analytical grade, Shantou Xilong Chemical Company, China, used as received.
(2) 99.5%, Analytical grade, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Propanol; C_3H_8O; [67-63-0]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables: T/K = 308.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2873\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical Source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical Source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7984	0.2016

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[75]F. A. Restaino and A. N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.797	0.203

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, shaker, analytical balance, constant-temperature bath, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials and allowed to equilibrate in a constant-temperature bath with shaking for 48 h. An aliquot of the equilibrated sample was removed and filtered. Concentration of the dissolved solute was determined gravimetrically and/or spectrophotometrically. The authors did not specify which of the two methods was used for the different solutes studied.

Source and Purity of Chemicals:
(1) Certified Reagent grade, Fisher Scientific, USA, was recrsytallized from trichloromethane.
(2) Certified Reagent grade, Fisher Scientific, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 239.7 mg/ml, which corresponds to a molar solubility of $c_1 = 1.963$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, UK, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ± 0.097.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8032	0.1968

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2529$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[91]J. Bradil, J. Malek, and V. Bazant, Chem. Prumysl **20**, 117 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
273.2	0.9355	0.0645
290.2	0.8915	0.1085
298.2	0.8596	0.1404
323.6	0.7545	0.2455
333.9	0.6824	0.3176
348.4	0.6147	0.3853
363.2	0.3878	0.6122

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were reported in terms of grams of dissolved solute per 100 g of solution. Mole fraction solubilities calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent and were placed in a flask and equilibrated at constant temperature with stirring. After 90 min the stirring was discontinued, and the solution was allowed to stand for 30 min to allow the undissolved solid to settle to the bottom of the flask. An aliquot of the saturated solution was removed by pipette fitted with a filtering device. The mass of the aliquot was determined by weighing. The concentration of the dissolved solute was determined by titration using sodium hydroxide, with phenolphthalein being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Argon, Lodz, Poland, no purification details were provided.
(2) Purity not given, Spolana, Neratovice, Czechoslovakia, was distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8476	0.1524

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.50 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) High Purity, National Bureau of Standards, USA, was dried *in vacuo* at 383 K before use.
(2) White Label, Eastman Kodak Chemical Company, Rochester, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.3092\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. 73, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8161	0.1839

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[75]F. A. Restaino and A. N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.774	0.226

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, shaker, analytical balance, constant-temperature bath, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials and allowed to equilibrate in a constant-temperature bath with shaking for 48 h. An aliquot of the equilibrated sample was removed and filtered. Concentration of the dissolved solute was determined gravimetrically and/or spectrophotometrically. The authors did not specify which of the two methods was used for the different solutes studied.

Source and Purity of Chemicals:
(1) Certified Reagent grade, Fisher Scientific, USA, was recrsytallized from trichloromethane.
(2) Certified Reagent grade, Fisher Scientific, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2919\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8095	0.1905

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[75]F. A. Restaino and A. N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.799	0.201

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, shaker, analytical balance, constant-temperature bath, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials and allowed to equilibrate in a constant-temperature bath with shaking for 48 h. An aliquot of the equilibrated sample was removed and filtered. Concentration of the dissolved solute was determined gravimetrically and/or spectrophotometrically. The authors did not specify which of the two methods was used for the different solutes studied.

Source and Purity of Chemicals:
(1) Certified Reagent grade, Fisher Scientific, USA, was recrsytallized from trichloromethane.
(2) Purity not given, Eastman Organic Chemicals, USA, was redistilled before use.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2301$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 3-Methyl-3-pentanol; $C_6H_{14}O$; [77-74-3]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7284	0.2716

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8054	0.1946

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and analytical balance. Very little experimental details were given in the paper. The solubility of the solute was by a weighing method.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Sigma Chemical Company, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±3.0% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2542$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8013	0.1987

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[75]F. A. Restaino and A. N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.871	0.129

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, shaker, analytical balance, constant-temperature bath, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials and allowed to equilibrate in a constant-temperature bath with shaking for 48 h. An aliquot of the equilibrated sample was removed and filtered. Concentration of the dissolved solute was determined gravimetrically and/or spectrophotometrically. The authors did not specify which of the two methods was used for the different solutes studied.

Source and Purity of Chemicals:
(1) Certified Reagent grade, Fisher Scientific, USA, was recrsytallized from trichloromethane.
(2) Purity not given, Eastman Organic Chemicals, USA, was redistilled before use.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[77]J. Qingzhu, M. Peisheng, Y. Shouzhi, W. Qiang, W. Chang, and L. Guiju, J. Chem. Eng. Data **53**, 1278 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.30	0.8335	0.1665
297.65	0.8199	0.1801
300.15	0.8078	0.1922
301.85	0.7967	0.2033
304.25	0.7886	0.2114
305.25	0.7806	0.2194
307.75	0.7726	0.2274
309.35	0.7650	0.2350
312.30	0.7501	0.2499
313.95	0.7345	0.2655
317.15	0.7207	0.2793
320.85	0.7103	0.2897
322.15	0.7000	0.3000

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating water bath, analytical balance, laser monitoring system. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate 0.5 K/20 min (0.2 K/20 min or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) <99%, Chemical source not specified, used as received.
(2) <99%, Chemical source not specified, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0005.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 152.6 mg/ml, which corresponds to a molar solubility of c_1 = 1.250 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, UK, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ± 0.078.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2674$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Nonanol; $C_9H_{20}O$; [143-08-8]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2439$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 123.8 mg/ml, which corresponds to a molar solubility of $c_1 = 1.014 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, UK, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ± 0.18.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[70]J. M. Jessy, J. Indian Chem. Soc. **75**, 352 (1998).
Variables:	**Prepared by:**
T/K = 308.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.2420 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. A convenient amount of benzoic acid in the form of fine powder was placed in a conical flask. Alcohol was added such that the volume was approximately half of that required to make the saturated solution. The flask was tightly stoppered and thermostated at 308 K for 15 min. Then, keeping the flask still partially immersed in the temperature bath, more alcohol was added dropwise with vigorous shaking by rotary motion until the last speck of solid dissolved. Repeated trials showed that the endpoint was quite reproducible. The experiment was performed a minimum of three times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].
(2) Purity not given, Chemical source not given, purification method was referenced to a published method [A. I. Vogel, *A Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis* (Longmans, London, 1968)].

Estimated Error:
Temperature: ±0.2 (estimated by compiler).
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzenemethanol; C_7H_8O; [100-51-6]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8559	0.1441

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9116	0.0884

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[78]A. Yurquina, M. E. Manzur, P. Brito, R. Manzo, and M. A. A. Molina, J. Mol. Liq. **108**, 119 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.501 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and an ultraviolet/visible spectrophotometer.
Very little experimental details were provided. Authors state that after equilibrium is obtained, the solution was filtered through Millipore filters having a porous size of 1 μm. Concentrations of the saturated solution were determined from spectroscopic measurements at an analysis wavelength of 227 nm.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ± 2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables: T/K = 305.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 240.8 mg/ml, which corresponds to a molar solubility of $c_1 = 1.972$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, UK, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.077.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[88]B. J. Aungst, J. A. Blake, and A. Hussain, Pharm. Res. **7**, 712 (1990).
Variables: T/K = Not given	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 250 mg/ml, which corresponds to a molar solubility of $c_1 = 2.047$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility measurements were performed as part of a study involving drug solubility, partitioning and skin permeation. There were very little experimental details given in regards to the solubility measurement. The authors simply state “Drug solubilities in the vehicles were determined after filtration and dilution or extraction.” For the skin permeation measurements the reservoir was maintained at 310 K. The solubility measurement may have been performed at 310 K as well.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific, USA, no purification details were provided.
(2) U.S.P. grade, Fisher Scientific, USA, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: Insufficient experimental details to estimate.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[61]E. R. Cooper, J. Controlled Release **1**, 153 (1984).
Variables: T/K = 295	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8652	0.1348

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Matheson, Coleman, and Bell, Cincinnati, OH, USA, no purification details provided.
(2) Reagent grade, J.T. Baker Chemical Company, Phillipsburg, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8464	0.1536

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[68]K. K. Kundu, A. L. De, and M. N. Das, J. Chem. Soc. Dalton Trans. **1972**, 386.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8300	0.1700

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details are given in paper. Authors state that a saturated solution can be obtained by mild shaking for approximately 24 h. Concentrations determined by titration with standard aqueous alkali.

Source and Purity of Chemicals:
(1) G.R. grade, Merck Chemical Company, was used as received.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,3-Propanediol; $C_3H_8O_2$; [504-63-2]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8826	0.1174

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2,3-Propanetriol (Glycerol); $C_3H_8O_3$; [56-81-5]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9836	0.0164

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1,2,3-Propanetriol (Glycerol); $C_3H_8O_3$; [56-81-5]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables: T/K = 305.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 22.60 mg/ml, which corresponds to a molar solubility of $c_1 = 0.185\ \mathrm{mol\ dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, ICN Biochemicals, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.0041.

2.8. Benzoic acid solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[62]S. H. Ghosh and D. K. Hazra, J. Chem. Soc., Perkin Trans. 2 **1989**, 1021.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $c_1 = 3.0535\ \mathrm{mol\ dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Mechanical shaker and a constant-temperature thermostat.
Excess solute and solvent were placed in a Campbell solubility apparatus and allowed to equilibrate at 298 K for 24 h. An aliquot of the saturated solution was then removed and filtered. The concentration of the dissolved solute was determined by titration with standard caustic soda using phenolphthalein as indicator. Solubility was also determined spectrophotometrically from absorbance measurements made at an analysis wavelength of 272 nm.

Source and Purity of Chemicals:
(1) G.R.E, Merck Chemical Company, was recrystallized from alcohol and then dried.
(2) Purity not given, Merck Chemical Company, was distilled twice before use.

Estimated Error:
Temperature: ±0.01 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7164	0.2836

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

2.9. Benzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Propanone; C_3H_6O; [67-64-1]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8143	0.1857

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Propanone; C_3H_6O; [67-64-1]	[69]C. M. McLoughlin, W. A. M. McMinn, and T. R. A. Magee, Powder Technol. **134**, 40 (2003).
Variables: T/K = 293	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 550 g/l. The authors did not specify whether the values were per liter of solvent or per liter of saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by adding (0.50 ± 0.1) g amounts of the powdered solute to (100 ± 1) ml of solvent until a saturated solution was obtained. The mass of the powder was recorded.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Poole, England, UK, no purification details were provided.
(2) Purity not given, Sigma-Aldrich, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
Solubility: ±5 g/l (estimated by compiler assuming solute added in increments of 0.50 g).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Propanone; C_3H_6O; [67-64-1]	[55]B. Long, J. Li, R. Zhang, and L. Wan, Fluid Phase Equilib. **297**, 113 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
277.59	0.8733	0.1267
282.21	0.8570	0.1430
287.03	0.8424	0.1576
287.19	0.8649	0.1571
293.20	0.8247	0.1753
298.15	0.8075	0.1925
302.95	0.7889	0.2111
307.75	0.7688	0.2312
313.05	0.7469	0.2531
317.63	0.7235	0.2765
322.72	0.6967	0.3033

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Double layer jacketed glass equilibrium cell, circulating water bath, analytical balance, and drying oven.
Excess solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was allowed to equilibrate at constant temperature with stirring for 3 h. The stirring was discontinued and the solution was allowed to stand for 1 h to allow the undissolved solid to settle to the bottom portion of the equilibrium vessel. An aliquot of the clear solution was transferred to a preweighed vial by a warm syringe. The vial was tightly closed and reweighed to determine the mass of the sample transferred. The vial was then put into a drying oven with the cap half-closed to permit complete evaporation of the solvent. The vial was covered with a piece of stainless steel filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was removed from the drying oven and placed in a desiccator with silica gel for another 2 h to reach ambient room temperature. The vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Analytical grade, Shantou Xilong Chemical Company, China, used as received.
(2) 99.5%, Analytical grade, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Propanone; C_3H_6O; [67-64-1]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1916).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.791	0.209

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath.
Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Propanone; C_3H_6O; [67-64-1]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7859	0.2141

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Acetophenone; C_8H_8O; [98-86-2]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8122	0.1878

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

2.10. Benzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9103	0.0897

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8919	0.1081

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Pyridine; C_5H_5N; [110-86-1]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.4652	0.5348

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8325	0.1675

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[55]B. Long, J. Li, R. Zhang, and L. Wan, Fluid Phase Equilib. **297**, 113 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
292.95	0.8715	0.1285
298.45	0.8519	0.1481
303.05	0.8345	0.1655
307.75	0.8345	0.1877
312.15	0.7893	0.2107
318.35	0.7633	0.2367
323.15	0.7338	0.2662
327.95	0.7033	0.2967
332.75	0.6719	0.3281
337.15	0.6464	0.3536
342.75	0.5992	0.4008
346.65	0.5750	0.4250

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Double layer jacketed glass equilibrium cell, circulating water bath, analytical balance, and drying oven.

Excess solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was allowed to equilibrate at constant temperature with stirring for 3 h. The stirring was discontinued and the solution was allowed to stand for 1 h to allow the undissolved solid to settle to the bottom portion of the equilibrium vessel. An aliquot of the clear solution was transferred to a preweighed vial by a warm syringe. The vial was tightly closed and reweighed to determine the mass of the sample transferred. The vial was then put into a drying oven with the cap half-closed to permit complete evaporation of the solvent. The vial was covered with a piece of stainless steel filter cloth to prevent dust contamination. After the solvent had evaporated the vial was removed from the drying oven and placed in a desiccator with silica gel for another 2 h to reach ambient room temperature. The vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:

(1) 99.5%, Analytical grade, Shantou Xilong Chemical Company, China, was used as received.

(2) 99.5%, Analytical grade, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:

Temperature: ±0.05 K.

x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[79]Q. Wang, L. Hou, Y. Cheng, and X. Li, J. Chem. Eng. Data **52**, 936 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.3	0.8903	0.1097
308.4	0.8689	0.1311
318.4	0.8424	0.1576
328.2	0.8199	0.1801
338.0	0.7928	0.2072
348.3	0.7753	0.2247
358.6	0.7446	0.2554

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

[c] Solubility data were given in units of grams per 100 g of solvent. Mole fraction solubilities were calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath and analytical balance.

Solubilities were determined by a static method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h. An aliquot of the clear solution was removed by syringe and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was evaporated in *in vacuo* at 323 K for more than 3 h. Once the solvent had evaporated, the vial with solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:

(1) 99%, Shanghai Fine Chemical Reagent Company, China, no purification details provided.

(2) Analytical Reagent grade, Hangzhou Chemical Reagent Company, China, no purification details provided.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[80]P. Ma and Q. Xia, Chin. J. Chem. Eng. **9**, 39 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
291.4	0.8709	0.1291
296.1	0.8559	0.1441
299.0	0.8456	0.1544
302.1	0.8336	0.1664
305.3	0.8252	0.1748
306.3	0.8191	0.1809
308.1	0.8130	0.1870
310.5	0.8005	0.1995
313.5	0.7874	0.2126
316.2	0.7753	0.2247
318.2	0.7616	0.2384
320.7	0.7494	0.2506
322.8	0.7359	0.2641
325.5	0.7226	0.2774
328.2	0.7061	0.2939
330.3	0.6923	0.3077
332.1	0.6806	0.3194
333.9	0.6684	0.3316

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system.

Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. Near the solid-liquid equilibrium temperature, the rate of temperature increase was 0.1 K/10 min. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Propanoic acid; $C_3H_6O_2$; [79-09-4]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8113	0.1887

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.4898	0.5102

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[81]A. G. Zakharov, M. I. Voronova, D. V. Batov, and K. V. Smirnova, Russ. J. Phys. Chem. **85**, 408 (2011).
Variables:	**Prepared by:**
T/K = 298	W. E. Acree, Jr.

Experimental Values

The authors reported the solubility data graphically. The compiler estimated a solubility of 14 molal (14 mol/kg of solvent) from the graph, which would correspond to a mole fraction solubility of $x_1 = 0.522$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. The authors stated that the solubility was determined at 298 K gravimetrically, and referenced a paper by Shalmashi and Eliassi [J. Chem. Eng. Data **53**, 199 (2008)].

Source and Purity of Chemicals:
(1) 99%, Sigma Aldrich Chemical Company, no purification details were provided.
(2) 99.5%, Lab-Scan, used as received.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ± 5 to 6% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[64]E. A. Gomaa, Phys. Chem. Liq. **50**, 279 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7165	0.2835

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute, computed by the compiler. The original solubility data were given in units of moles per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature shaker bath and analytical balance.
Excess solute and solvent were placed in closed test tubes and allowed to equilibrate in a constant-temperature shaker bath for several days. The solubility was determined gravimetrically by transferring 1 ml of the saturated solution to an aluminum disk. The solvent was removed by heating with an infrared lamp. The solubility was calculated from the mass of the solid residue and amount of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.
(2) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Formamide; CH_3NO; [75-12-7]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8475	0.1525

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) *N*-Methylformamide; C_2H_5NO; [123-39-7]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6572	0.3428

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.5091	0.4909

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath and ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, no information provided concerning purification.

(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3% (relative error).

Components:

(1) Benzoic acid; $C_7H_6O_2$; [65-85-0]

(2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]

Original Measurements:

[64]E. A. Gomaa, Phys. Chem. Liq. **50**, 279 (2012).

Variables:

T/K = 298.15

Prepared by:

W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7772	0.2228

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute, computed by the compiler. The original solubility data were given in units of moles per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature shaker bath and analytical balance.

Excess solute and solvent were placed in closed test tubes and allowed to equilibrate in a constant-temperature shaker bath for several days. The solubility was determined gravimetrically by transferring 1 ml of the saturated solution to an aluminum disk. The solvent was removed by heating with an infrared lamp. The solubility was calculated from the mass of the solid residue and amount of saturated solution analyzed.

Source and Purity of Chemicals:

(1) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

(2) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

x_1: ±3% (relative error, estimated by compiler).

Components:

(1) Benzoic acid; $C_7H_6O_2$; [65-85-0]

(2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]

Original Measurements:

[80]P. Ma and Q. Xia, Chin. J. Chem. Eng. **9**, 39 (2001).

Variables:

Temperature

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.8	0.5276	0.4724
300.7	0.5227	0.4773
301.1	0.5224	0.4776
302.7	0.5190	0.4810
304.6	0.5161	0.4839
306.3	0.5119	0.4881
308.2	0.5088	0.4912
310.1	0.5043	0.4957
312.2	0.4996	0.5004
316.5	0.4896	0.5104
319.4	0.4824	0.5176
321.8	0.4762	0.5238
323.4	0.4719	0.5281
325.7	0.4662	0.5338
329.1	0.4572	0.5428
331.6	0.4480	0.5520
334.3	0.4416	0.5584
336.4	0.4358	0.5642
340.1	0.4226	0.5774
343.1	0.4098	0.5902

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system.

Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. Near the solid-liquid equilibrium temperature, the rate of temperature increase was 0.1 K per 10 min. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

x_1: ±3% (relative error, estimated by compiler).

Components:

(1) Benzoic acid; $C_7H_6O_2$; [65-85-0]

(2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]

Original Measurements:

[82]L. Dian-Qing, L. Jiang-Chu, L. Da-Zhuang, and W. Fu-An, Fluid Phase Equilib. **200**, 69 (2002).

Variables:

Temperature

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
294.75	0.5357	0.4643
298.75	0.5273	0.4727
301.05	0.5224	0.4776
302.15	0.5186	0.4814
306.35	0.5119	0.4881
310.05	0.5043	0.4957
312.15	0.4996	0.5004
316.55	0.4896	0.5104
319.35	0.4824	0.5176
323.35	0.4719	0.5281
325.65	0.4662	0.5338
329.05	0.4572	0.5428
331.85	0.4480	0.5520
336.45	0.4336	0.5664
340.05	0.4226	0.5774
343.35	0.4098	0.5902
346.05	0.3985	0.6015
348.75	0.3865	0.6135
351.25	0.3757	0.6243
355.55	0.3528	0.6472
358.05	0.3395	0.6605
362.85	0.3129	0.6871
366.85	0.2874	0.7126
369.65	0.2665	0.7335

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) Analytical Reagent, Shanghai Chemical Reagent Company, China, used as received.
(2) Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 5.35 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) High purity, National Bureau of Standards, USA, no purification details given.
(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[47]A. Beerbower, P. L. Wu, and A. Martin, J. Pharm. Sci. **73**, 179 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.4755	0.5245

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9461	0.0539

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and analytical balance. Very little experimental details were given in the paper. The solubility of the solute was by a weighing method.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) HPLC grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±3.0% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[64]E. A. Gomaa, Phys. Chem. Liq. **50**, 279 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9577	0.0423

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute, computed by the compiler. The original solubility data were given in units of moles per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature shaker bath and analytical balance.
Excess solute and solvent were placed in closed test tubes and allowed to equilibrate in a constant-temperature shaker bath for several days. The solubility was determined gravimetrically by transferring 1 ml of the saturated solution to an aluminum disk. The solvent was removed by heating with an infrared lamp. The solubility was calculated from the mass of the solid residue and amount of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.
(2) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15 K	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.85 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) High Purity, National Bureau of Standards, USA, was dried at 383 K before use.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[81]A. G. Zakharov, M. I. Voronova, D. V. Batov, and K. V. Smirnova, Russ. J. Phys. Chem. **85**, 408 (2011).
Variables: T/K = 298	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The authors reported the solubility data graphically. The compiler estimated a solubility of 1 molal (1 mol/kg of solvent) from the graph, which would correspond to a mole fraction solubility of $x_1 = 0.0394$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. The authors stated that the solubility was determined at 298 K gravimetrically, and referenced a paper by Shalmashi and Eliassi [J. Chem. Eng. Data **53**, 199 (2008)].

Source and Purity of Chemicals:
(1) 99%, Sigma Aldrich Chemical Company, no purification details were provided.
(2) 99.9%, Lab-Scan, used as received.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ± 5 to 6% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Hexamethylphosphortriamide; $C_6H_{18}N_3OP$; [680-31-9]	[64]E. A. Gomaa, Phys. Chem. Liq. **50**, 279 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9857	0.0143

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute, computed by the compiler. The original solubility data were given in units of moles per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature shaker bath and analytical balance.
Excess solute and solvent were placed in closed test tubes and allowed to equilibrate in a constant-temperature shaker bath for several days. The solubility was determined gravimetrically by transferring 1 ml of the saturated solution to an aluminum disk. The solvent was removed by heating with an infrared lamp. The solubility was calculated from the mass of the solid residue and amount of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.
(2) Purity not given, Merck Chemicals, Germany, no information provided concerning purification.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[84]D.-Q. Li, D.-Z. Liu, and F.-A. Wang, J. Chem. Eng. Data **46**, 172 (2001).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.35	0.4838	0.5162
301.15	0.4765	0.5235
305.05	0.4698	0.5302
307.95	0.4647	0.5353
311.05	0.4591	0.5409
314.25	0.4530	0.5470
318.35	0.4465	0.5535
321.95	0.4393	0.5607
327.35	0.4256	0.5744
333.55	0.4087	0.5913
338.85	0.3918	0.6082
343.25	0.3772	0.6228
347.75	0.3605	0.6395
351.15	0.3465	0.6535
355.05	0.3309	0.6691
359.85	0.3067	0.6933
364.55	0.2819	0.7181
369.05	0.2553	0.7447
371.35	0.2408	0.7592

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system.
Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) 99.5%, Analytical Reagent, Shanghai Chemical Reagent Company, China, used as received.
(2) 99.0%, Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Ethyl 2-hydroxypropanoate; $C_5H_{10}O_3$; [97-64-3]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 164.70 mg/ml, which corresponds to a molar solubility of c_1 = 1.349 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Purac Biochem, Gorinchem, Netherlands, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.20.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 1-Methylethyl 2-hydroxypropanoate; $C_6H_{12}O_3$; [617-64-3]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 239.70 mg/ml, which corresponds to a molar solubility of c_1 = 1.963 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Purac Biochem, Gorinchem, Netherlands, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.095.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Butyl 2-hydroxypropanoate; $C_7H_{14}O_3$; [138-22-7]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 135.80 mg/ml, which corresponds to a molar solubility of c_1 = 1.112 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Purac Biochem, Gorinchem, Netherlands, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ± 0.038.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Butyl 2-hydroxypropanoate; $C_7H_{14}O_3$; [128-22-7]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7987	0.2013

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Purity not given, Purac Inc., no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) γ-Butyrolactone; $C_4H_6O_2$; [96-48-0]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8434	0.1566

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Dimethyl isosorbide; $C_8H_{14}O_4$; [5306-85-4]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6810	0.3190

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Amend Drug and Chemical Company, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 9(Z)-Octadecenoic acid (Oleic acid); $C_{18}H_{34}O_2$; [112-80-1]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 245.50 mg/ml, which corresponds to a molar solubility of $c_1 = 2.010$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisons Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ± 0.16.

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Furancarboxylic acid; $C_5H_4O_3$; [88-14-2]	[85]K. Mislow, J. Phys. Colloid Chem. **52**, 729 (1948).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

t/°C (thawing)	t/°C (melting)	w_1[a]
132	133	0.000
85.6	127.2	0.104
85.1	124.0	0.217
85.0	121.5	0.289
85.3	114.5	0.420
85.5	100.2	0.486
85.0	95.2	0.570
85.0	96.0	0.669
85.1	105.5	0.775
85.1	110.8	0.865
121	122	1.000

[a]w_1: mass fraction solubility of the solute.

The author reports that the binary system forms a simple eutectic at $w_1 = 0.600$ and $t = 85$ °C.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental method involved observing the thawing-melting behavior of binary mixtures of known composition. Thoroughly mixed samples were placed in capillaries, and sealed at one end. The capillaries were placed next to the junction of a thermocouple in a hot stage, which was mounted on a polarizing microscope. Heating rates were kept at (2 ± 1) °C/min. The thawing temperature was observed by reflected light, while the melting points were observed by transmitted light. Accuracy of the method, as judged by the reproducibility of the measured data, was estimated to be ± 2 °C for thawing and melting temperatures.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, recrystallized from aqueous solution.
(2) Purity not given, Chemical source not given, recrystallized from aqueous solution.

Estimated Error:
Temperature: 2 °C.
w_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Pyridinecarboxylic acid; $C_6H_5NO_2$; [98-98-6]	[85]K. Mislow, J. Phys. Colloid Chem. **52**, 729 (1948).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

t/°C (thawing)	t/°C (melting)	w_1[a]
136	137	0.000
88.4	134.2	0.116
87.6	131.0	0.186
86.4	123.8	0.303
87.0	116.0	0.383
87.2	107.4	0.465
87.4	102.4	0.588
87.0	107.4	0.672
87.6	111.4	0.755
87.6	116.2	0.866
121	122	1.000

[a]w_1: mass fraction solubility of the solute.

The author reports that the binary system forms a simple eutectic at $w_1 = 0.530$ and $t = 115$ °C.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental method involved observing the thawing-melting behavior of binary mixtures of known composition. Thoroughly mixed samples were placed in capillaries, and sealed at one end. The capillaries were placed next to the junction of a thermocouple in a hot stage, which was mounted on a polarizing microscope. Heating rates were kept at (2 ± 1) °C/min. The thawing temperature was observed by reflected light, while the melting points were observed by transmitted light. Accuracy of the method, as judged by the reproducibility of the measured data, was estimated to be ± 2 °C for thawing and melting temperatures.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, recrystallized from aqueous solution.
(2) Purity not given, Chemical source not given, recrystallized from aqueous solution.

Estimated Error:
Temperature: 2 °C.
w_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 3-Pyridinecarboxylic acid; $C_6H_5NO_2$; [59-67-6]	[85]K. Mislow, J. Phys. Colloid Chem. **52**, 729 (1948).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

t/°C (thawing)	t/°C (melting)	w_1[a]
233	233	0.000
115.0	227.6	0.090
115.4	217.6	0.200
115.4	211.2	0.286
114.2	195.8	0.454
115.0	184.0	0.505
114.6	169.8	0.666
114.0	142.2	0.708
113.6	117.8	0.890
114.0	120.4	0.968
121	122	1.000

[a]w_1: mass fraction solubility of the solute.

The author reports that the binary system forms a simple eutectic at $w_1 = 0.900$ and $t = 115$ °C.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental method involved observing the thawing-melting behavior of binary mixtures of known composition. Thoroughly mixed samples were placed in capillaries, and sealed at one end. The capillaries were placed next to the junction of a thermocouple in a hot stage, which was mounted on a polarizing microscope. Heating rates were kept at (2 ± 1) °C/min. The thawing temperature was observed by reflected light, while the melting points were observed by transmitted light. Accuracy of the method, as judged by the reproducibility of the measured data, was estimated to be ± 2 °C for thawing and melting temperatures.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, recrystallized from aqueous solution.
(2) Purity not given, Chemical source not given, recrystallized from aqueous solution.

Estimated Error:
Temperature: 2 °C.
w_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 4-Pyridinecarboxylic acid; $C_6H_5NO_2$; [55-22-1]	[85]K. Mislow, J. Phys. Colloid Chem. **52**, 729 (1948).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

t/°C (thawing)	t/°C (melting)	w_1[a]
312	314 (decomposed)	0.000
11.6	304 (decomposed)	0.081
115.4	282.8	0.368
115.0	265.4	0.539
115.0	264.2	0.618
115.0	255.4	0.684
114.8	225.2	0.818
115.4	199.4	0.894
115.4	158.8	0.961
121	122	1.000

[a]w_1: mass fraction solubility of the solute.

The author reports that the binary system forms a simple eutectic at $w_1 = 0.990$ and $t = 115$ °C.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental method involved observing the thawing-melting behavior of binary mixtures of known composition. Thoroughly mixed samples were placed in capillaries, and sealed at one end. The capillaries were placed next to the junction of a thermocouple in a hot stage, which was mounted on a polarizing microscope. Heating rates were kept at (2 ± 1) °C/min. The thawing temperature was observed by reflected light, while the melting points were observed by transmitted light. Accuracy of the method, as judged by the reproducibility of the measured data, was estimated to be ± 2 °C for thawing and melting temperatures.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, recrystallized from aqueous solution.
(2) Purity not given, Chemical source not given, recrystallized from aqueous solution.

Estimated Error:
Temperature: 2 °C.
w_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) 2-Thiophenecarboxylic acid; $C_5H_4O_2S$; [527-72-0]	[85]K. Mislow, J. Phys. Colloid Chem. **52**, 729 (1948).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

t/°C (thawing)	t/°C (melting)	w_1[a]
127	128	0.000
94.6	123.8	0.084
94.8	120.4	0.171
94.8	118.6	0.207
95.4	115.2	0.308
94.8	112.0	0.383
95.8	110.2	0.415
95.2	109.2	0.445
95.4	104.8	0.555
94.4	109.2	0.710
94.8	111.6	0.767
95.6	116.2	0.835
95.6	117.0	0.860
97.8	120.6	0.903
121	122	1.000

[a] w_1: mass fraction solubility of the solute.

The author reports that the binary system forms a simple eutectic at $w_1 = 0.630$ and $t = 95$ °C, with an indication of solid solution formation at $w_1 > 0.90$.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental method involved observing the thawing-melting behavior of binary mixtures of known composition. Thoroughly mixed samples were placed in capillaries, and sealed at one end. The capillaries were placed next to the junction of a thermocouple in a hot stage, which was mounted on a polarizing microscope. Heating rates were kept at (2 ± 1) °C/min. The thawing temperature was observed by reflected light, while the melting points were observed by transmitted light. Accuracy of the method, as judged by the reproducibility of the measured data, was estimated to be ±2 °C for thawing and melting temperatures.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, recrystallized from aqueous solution.
(2) Purity not given, prepared by the authors, synthesized by iodinating thiophene, and then converting the resulting 2-iodothiophene into the desired acid by the Grignard synthesis. The sample was purified by successive recrystallizations from aqueous solution and from ligroin-benzene mixture.

Estimated Error:
Temperature: 2 °C.
w_1: ±0.002 (estimated by compiler).

2.11. Benzoic acid solubility data in binary organic solvent mixtures

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Hexane; C_6H_{14}; [110-54-3]	[49] W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables:	**Prepared by:**
Temperature; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	$x_2^{(s)}$[a]	x_1[b]
298.15	0.0000	0.0100
298.15	0.2573	0.0108
298.15	0.4699	0.0113
298.15	0.5342	0.0115
298.15	0.6566	0.0118
298.15	0.8044	0.0117
298.15	1.0000	0.0115
303.15	0.0000	0.0126
303.15	0.2341	0.0136
303.15	0.2845	0.0138
303.15	0.5059	0.0146
303.15	0.6670	0.0150
303.15	0.7821	0.0151
303.15	1.0000	0.0146

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99+%, Chemical source not given, was dried over molecular sieves and distilled before use.
(3) 99%, Chemical source not given, was dried over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Heptane; C_7H_{16}; [142-82-5]	[49] W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
0.0000	0.0000	0.0114
0.2781	0.2748	0.0119
0.4602	0.4546	0.0121
0.5713	0.5644	0.0121
0.6825	0.4742	0.0122
0.8142	0.4045	0.0119
1.0000	0.9885	0.0115

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99+%, Chemical source not given, was dried over molecular sieves and distilled before use.
(3) 99+%, Chemical source not given, was dried over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1% (relative error).

Components:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0]
(2) Hexane; C_6H_{14}; [110-54-3]
(3) Tetrachloromethane; CCl_4; [56-23-5]

Original Measurements:
[49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).

Variables:
Temperature; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	$x_2^{(s)}$[a]	x_1[b]
298.15	0.0000	0.0492
298.15	0.1550	0.0395
298.15	0.3419	0.0297
298.15	0.4408	0.0251
298.15	0.5951	0.0195
298.15	0.8028	0.0137
298.15	1.0000	0.0100
303.15	0.0000	0.0598
303.15	0.2255	0.0483
303.15	0.3078	0.0391
303.15	0.4556	0.0304
303.15	0.6438	0.0226
303.15	0.7564	0.0185
303.15	1.0000	0.0126

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99%, Chemical source not given, was dried over molecular sieves and distilled before use.
(3) 99+%, Chemical source not given, refluxed for 11 h over an aqueous solution 10% in potassium permanganate and 10% in sodium hydroxide. The tetrachloromethane was distilled off and dried with calcium hydroxide, stored in contact with mercury under an argon atmosphere, and then distilled shortly before use.

Estimated Error:
Temperature: ±0.01 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1% (relative error).

Components:
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0]
(2) Heptane; C_7H_{16}; [142-82-5]
(3) Tetrachloromethane; CCl_4; [56-23-5]

Original Measurements:
[49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).

Variables:
Temperature; Solvent Composition

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	$x_2^{(s)}$[a]	x_1[b]
298.15	0.0000	0.0492
298.15	0.1784	0.0375
298.15	0.2303	0.0347
298.15	0.3348	0.0295
298.15	0.3930	0.0270
298.15	0.3932	0.0269
298.15	0.4708	0.0240
298.15	0.5433	0.0214
298.15	0.7013	0.0170
298.15	1.0000	0.0114
303.15	0.0000	0.0598
303.15	0.2421	0.0423
303.15	0.4269	0.0322
303.15	0.6237	0.0241
303.15	0.7346	0.0206
303.15	1.0000	0.0147

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99+%, Chemical source not given, was dried over molecular sieves and distilled before use.
(3) 99+%, Chemical source not given, refluxed for 11 h over an aqueous solution 10% in potassium permanganate and 10% in sodium hydroxide. The tetrachloromethane was distilled off and dried with calcium hydroxide, stored in contact with mercury under an argon atmosphere, and then distilled shortly before use.

Estimated Error:
Temperature: ±0.01 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Tetrachloromethane; CCl_4; [56-23-5]	[49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
0.0000	0.0000	0.0492
0.1847	0.1775	0.0389
0.3681	0.3568	0.0307
0.5207	0.5079	0.0246
0.6226	0.6094	0.0212
0.8084	0.7958	0.0156
1.0000	0.9885	0.0115

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was dried at 333 K for several hours before use.
(2) 99+%, Chemical source not given, was dried over molecular sieves and distilled before use.
(3) 99+%, Chemical source not given, refluxed for 11 h over an aqueous solution 10% in potassium permanganate and 10% in sodium hydroxide. The tetrachloromethane was distilled off and dried with calcium hydroxide, stored in contact with mercury under an argon atmosphere, and then distilled shortly before use.

Estimated Error:
Temperature: ±0.01 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Heptane; C_7H_{16}; [142-82-5] (3) Ethanol; C_2H_6O; [64-17-5]	[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).
Variables:	**Prepared by:**
Temperature; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	$m_2^{(s)a}$	x_1^b
278.15	0.00	0.128
278.15	0.10	0.121
278.15	0.20	0.112
278.15	0.30	0.102
278.15	0.40	0.092
278.15	0.50	0.079
278.15	1.00	0.005
283.15	0.00	0.139
283.15	0.10	0.132
283.15	0.20	0.123
283.15	0.30	0.111
283.15	0.40	0.101
283.15	0.50	0.087
283.15	1.00	0.006
293.15	0.00	0.166
293.15	0.10	0.158
293.15	0.20	0.147
293.15	0.30	0.135
293.15	0.40	0.124
293.15	0.50	0.107
293.15	1.00	0.010
303.15	0.00	0.196
303.15	0.10	0.188
303.15	0.20	0.178
303.15	0.30	0.164
303.15	0.40	0.145
303.15	0.50	0.132
303.15	1.00	0.015
313.15	0.00	0.234
313.15	0.10	0.227
313.15	0.20	0.216
313.15	0.30	0.203
313.15	0.40	0.187
313.15	0.50	0.165
313.15	1.00	0.022
323.15	0.00	0.276
323.15	0.10	0.271
323.15	0.20	0.261
323.15	0.30	0.246
323.15	0.40	0.224
323.15	0.50	0.203
323.15	1.00	0.033

[a] $m_2^{(s)}$: initial mass fraction of component 2 in the binary solvent mixture.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.

Solubilities were determined by a gravimetric method. Binary solvent mixtures were prepared by mass and allowed to equilibrate in sealed bottles in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:

(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 99%, VWR Scientific, USA, used as received.
(3) 99+%, Solveco Chemicals, used as received.

Estimated Error:

Temperature: ±0.01 K.
$m_2^{(s)}$: ±0.01.
x_1: ±1% (relative error).

Components:

(1) Benzoic acid; $C_7H_6O_2$; [65-85-0]
(2) Methylbenzene; C_7H_8; [108-88-3]
(3) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:

[48]J. Thati, F. L. Nordström, and A. C. Rasmuson, J. Chem. Eng. Data **55**, 5124 (2010).

Variables:

Temperature; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	$m_2^{(s)a}$	x_1^b
278.15	0.00	0.128
278.15	0.10	0.127
278.15	0.20	0.125
278.15	0.30	0.123
278.15	0.40	0.119
278.15	0.50	0.112
278.15	1.00	0.035
283.15	0.00	0.139
283.15	0.10	0.138
283.15	0.20	0.137
283.15	0.30	0.133
283.15	0.40	0.129
283.15	0.50	0.122
283.15	1.00	0.043
293.15	0.00	0.166
293.15	0.10	0.163
293.15	0.20	0.161
293.15	0.30	0.157
293.15	0.40	0.152
293.15	0.50	0.145
293.15	1.00	0.062
303.15	0.00	0.196
303.15	0.10	0.194
303.15	0.20	0.191
303.15	0.30	0.186
303.15	0.40	0.181
303.15	0.50	0.172
303.15	1.00	0.089
313.15	0.00	0.234
313.15	0.10	0.231
313.15	0.20	0.227
313.15	0.30	0.222
313.15	0.40	0.214
313.15	0.50	0.203
313.15	1.00	0.128
323.15	0.00	0.276
323.15	0.10	0.273
323.15	0.20	0.266
323.15	0.30	0.262
323.15	0.40	0.254
323.15	0.50	0.234
323.15	1.00	0.178

[a] $m_2^{(s)}$: initial mass fraction of component 2 in the binary solvent mixture.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.

Solubilities were determined by a gravimetric method. Binary solvent mixtures were prepared by mass and allowed to equilibrate in sealed bottles in a constant-temperature bath for 2 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. After 30 min, an aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:

(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 99+%, Merck Chemical Company, used as received.
(3) 99+%, Solveco Chemicals, used as received.

Estimated Error:

Temperature: ±0.01 K.
$m_2^{(s)}$: ±0.01.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Trichloromethane; $CHCl_3$; [67-66-3] (3) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1917).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$w_2^{(s)\,a}$	$s_1^{\,b}$	$m_1^{\,c}$
0.00	15.0	1.228
0.10	15.2	1.245
0.20	15.6	1.277
0.40	18.6	1.523
0.60	23.2	1.900
0.80	30.1	2.465
0.90	34.0	2.784
1.00	38.4	3.144

[a] $w_2^{(s)}$: initial mass fraction of component 2 in the binary solvent mixture.
[b] s_1: solubility of the solute given as grams of solute per 100 g of solvent.
[c] m_1: solubility of the solute given as moles of solute per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature thermostat, analytical balance, and a steam bath.

Binary solvent mixtures were prepared by mass. Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, purification details were not provided.
(2) Purity not given, Chemical source not given, purification details were not provided.
(3) Purity not given, Chemical source not given, purification details were not provided.

Estimated Error:

Temperature: ±0.1 K.
$w_2^{(s)}$: ±0.01.
m_1: ±10% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2] (3) Propanone; C_3H_6O; [67-64-1]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1917).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$w_2^{(s)\,a}$	$s_1^{\,b}$	$m_1^{\,c}$
0.00	55.6	4.553
0.10	51.3	4.201
0.20	49.2	4.029
0.40	42.2	3.456
0.60	33.5	2.743
0.80	24.1	1.973
0.90	18.3	1.499
1.00	11.6	0.950

[a] $w_2^{(s)}$: initial mass fraction of component 2 in the binary solvent mixture.
[b] s_1: solubility of the solute given as grams of solute per 100 g of solvent.
[c] m_1: solubility of the solute given as moles of solute per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature thermostat, analytical balance, and a steam bath.

Binary solvent mixtures were prepared by mass. Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, purification details were not provided.
(2) Purity not given, Chemical source not given, purification details were not provided.
(3) Purity not given, Chemical source not given, purification details were not provided.

Estimated Error:
Temperature: ±0.1 K.
$w_2^{(s)}$: ±0.01.
m_1: ±10% (relative error).

Components:	**Original Measurements:**
(1) Benzoic acid; $C_7H_6O_2$; [65-85-0] (2) Benzene; C_6H_6; [71-43-2] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[57]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **38**, 1235 (1917).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$w_2^{(s)}$[a]	s_1[b]	m_1[c]
0.00	41.2	3.374
0.10	28.1	2.301
0.20	29.0	2.375
0.40	23.9	1.957
0.60	20.4	1.670
0.80	16.5	1.351
0.90	14.0	1.146
1.00	11.6	0.950

[a] $w_2^{(s)}$: initial mass fraction of component 2 in the binary solvent mixture.
[b] s_1: solubility of the solute given as grams of solute per 100 g of solvent.
[c] m_1: solubility of the solute given as moles of solute per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath. Binary solvent mixtures were prepared by mass. Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification details were not provided.
(2) Purity not given, Chemical source not given, purification details were not provided.
(3) Purity not given, Chemical source not given, purification details were not provided.

Estimated Error:
Temperature: ±0.1 K.
$w_2^{(s)}$: ±0.01.
m_1: ±10% (relative error).

3. Solubility of 2-Acetoxybenzoic Acid in Organic Solvents

3.1. Critical evaluation of experimental solubility data

There have been several published studies[12,53,69,92–94] investigating the solubility behavior of 2-acetoxybenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Charlton *et al.*[12] measured the solubility of 2-acetoxybenzoic acid in 19 alcohols (1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 2-methyl-2-butanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, 2-ethyl-1-hexanol, 1-decanol, and 3,7-dimethyl-1-octanol), in four dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, 1,1′-oxybisbutane, and 2-methoxy-2-methylpropane (also called methyl *tert*-butyl ether) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in five alkyl alkanoates (methyl ethanoate, ethyl ethanoate, butyl ethanoate, pentyl ethanoate and methyl butanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to update the existing Abraham solute descriptors that the authors had for 2-acetoxybenzoic acid. The authors were able to assemble a total of 44 $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 2-acetoxybenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -1.68$.[95] The McGowan volume of 2-acetoxybenzoic acid, $V = 1.2879$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.780$. This left four solute descriptors (S, A, B, and L) still to be determined. The 44 equations were then solved using the Microsoft “SOLVER” program to yield numerical values of the remaining four solute descriptors, $S = 1.690$, $A = 0.710$, $B = 0.670$, and $L = 6.2789$, that best described the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -10.18$ for the gas-phase solute concentration that made the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) predictions internally consistent. The calculated molecular solute descriptors reproduced the 44 combined $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values to within an average standard deviation of 0.129 $\log_{10}$ units. The authors excluded 2-methoxy-2-methylpropane from the standard deviation computations because of concerns that trace water in the solvent might adversely affect the measured solubility. Diaz and Drogos[96] reported that 2-methoxy-2-methylpropane has limited stability in water acidified with either mineral acids or organic acids. The authors noted that the reaction proceeds even in very dilute solutions with weak acids, such as acetylsalicylic acid. The reaction produces methanol, which would enhance the saturation solubility. Acetylsalicylic acid is more soluble in methanol than in 2-methoxy-2-methylpropane. Such chemical

TABLE 8. Comparison between observed and calculated molar solubilities of 2-acetoxybenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\text{exp}}$	$\log_{10} c_1^{\text{calc}}$; Eq. (20)	$\log_{10} c_1^{\text{calc}}$; Eq. (21)
Methanol	0.176[a]	0.169	−0.248
Ethanol	0.114[a]	−0.050	−0.004
1-Propanol	−0.197	−0.179	−0.179
2-Propanol	−0.186	−0.167	−0.153
1-Butanol	−0.324	−0.314	−0.301
2-Butanol	−0.256	−0.195	−0.237
2-Methyl-1-propanol	−0.471	−0.366	−0.361
2-Methyl-2-propanol	−0.154	−0.146	−0.147
1-Pentanol	−0.443	−0.426	−0.427
2-Pentanol	−0.404	−0.411	−0.384
3-Methyl-1-butanol	−0.462	−0.436	−0.399
1-Hexanol	−0.505	−0.455	−0.468
1-Heptanol	−0.565	−0.478	−0.519
1-Octanol	−0.665	−0.519	−0.633
1-Decanol	−0.718	−0.739	−0.767
1,1′-Oxybisethane	−0.478	−0.572	−0.503
Tetrahydrofuran	0.312	0.435	0.363
1,4-Dioxane	0.134	0.316	0.307
Methyl ethanoate	−0.192	−0.061	−0.061
Ethyl ethanoate	−0.351	−0.255	−0.245
Butyl ethanoate	−0.597	−0.435	−0.456
Propanone	0.017[a]	0.133	0.184

[a] Experimental solubility data taken from Perlovich and Bauer-Brandl.[53] All other experimental data were taken from Charlton *et al.*[12]

TABLE 9. Parameters of the Modified Apelblat equation for describing the solubility of 2-acetoxybenzoic acid in various organic solvents[a]

Solvent	T/K	A	B	C	APLD (%)
Ethanol	276–336	63.952	−5759.6	−8.323	0.679
2-Propanol	282–330	588.32	−30787.7	−85.663	3.372
1,2-Propanediol	296–334	477.25	−27072.7	−68.500	0.674
Propanone	282–326	588.32	257.07	8.125	0.550

[a] Values of the coefficients and average percent logarithmic deviation were taken from Maia and Giulietti.[92]

reaction effects are expected to be fairly small if water is needed for the reaction to proceed.

After the 2-acetoxybenzoic acid solubility study was published, Abraham model correlations have been developed for 3-methyl-1-butanol, 2-pentanol, methyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 2-acetoxybenzoic acid solubility data. Table 8 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 2-acetoxybenzoic acid, x_1, determined by Charlton *et al.*[12] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\text{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\text{solvent}}]$). The molar volume of the hypothetical subcooled liquid 2-acetoxybenzoic acid is $V_{\text{solute}} = 126.89\ \text{cm}^3\ \text{mol}^{-1}$. Examination of the numerical entries in Table 8 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Independent 2-acetoxybenzoic acid solubility measurements do exist for several solvents. Previously Perlovich and Bauer-Brandl[53] had measured the solubility of 2-acetoxybenzoic acid in eight 1-alkanols (methanol through 1-octanol), and in benzene, methylbenzene, ethyl ethanoate, 1,4-dioxane, trichloromethane, propanone, and ethanenitrile. Except for 1,4-dioxane, the two sets of solubility data are in reasonably good agreement for the most part, $x_1 = 0.04976$ (Ref. 91) versus $x_1 = 0.0418$ (Ref. 53) for 1-propanol, $x_1 = 0.04616$ (Ref. 12) versus $x_1 = 0.0453$ (Ref. 53) for 1-butanol, $x_1 = 0.03966$ (Ref. 91) versus $x_1 = 0.0395$ (Ref. 53) for 1-pentanol, $x_1 = 0.03973$ (Ref. 12) versus $x_1 = 0.0393$ (Ref. 53) for 1-hexanol, $x_1 = 0.03892$ (Ref. 12) versus $x_1 = 0.0386$ (Ref. 53) for 1-heptanol, $x_1 = 0.03581$ (Ref. 12) versus $x_1 = 0.0341$ (Ref. 53) for 1-octanol, $x_1 = 0.04583$ (Ref. 12) versus $x_1 = 0.0448$ (Ref. 53) for ethyl ethanoate, and $x_1 = 0.1263$ (Ref. 12) versus $x_1 = 0.0516$ (Ref. 53) for 1,4-dioxane. Differences in chemical purities and experimental methodologies can lead to differences of a few percent between values determined by two different research groups.

There has been one experimental study examining the solubility of 2-acetoxybenzoic acid as a function of temperature. Maina and Giulietti[92] measured the solubility of 2-acetoxybenzoic acid in ethanol, 2-propanol, 1,2-propanediol, and propanone at several temperatures in the range of about 280–330 K. The internal consistency of the datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 9, along with the average percent logarithmic deviation (APLD) calculated according to

$$\text{APLD} = \frac{100}{N}\sum_{i=1}^{N}\left|\ln\left(\frac{x_i^{\text{exp}}}{x_i^{\text{calc}}}\right)\right|, \tag{26}$$

where N is the number of experimental solubility measurements in an individual solute-solvent dataset. Examination of the numerical entries in the last column of Table 9 reveals that the largest APLD between the back-calculated values based on Eq. (8) and experimental data is 3.5%. Results of the mathematical representation analyses indicate that the experimental data for all four 2-acetoxybenzoic acid – organic solvent systems are internally consistent.

The experimental solubility data for 2-acetoxybenzoic acid in organic solvents are in Secs. 3.2–3.8.

3.2. 2-Acetoxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Benzene; C_6H_6; [71-43-2]	[53] G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9990	0.00101

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Methylbenzene; C_7H_8; [108-88-3]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9987	0.00129

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

3.3. 2-Acetoxybenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9471	0.05287

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9542	0.04583

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9552	0.0448

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9665	0.03345

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9732	0.02677

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Methyl butanoate; $C_5H_{10}O_2$; [623-42-7]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9703	0.02970

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

3.4. 2-Acetoxybenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9647	0.03529

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9878	0.01224

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9929	0.007095

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9599	0.04013

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8096	0.1904

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8737	0.1263

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9484	0.0516

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Sigma Chemical Company, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

3.5. 2-Acetoxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.794	0.206

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

3.6. 2-Acetoxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Methanol; CH_4O; [67-56-1]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9281	0.0719

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) HPLC grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Methanol; CH_4O; [67-56-1]	[69]C. M. McLoughlin, W. A. M. McMinn, and T. R. A. Magee, Powder Technol. **134**, 40 (2003).
Variables:	**Prepared by:**
T/K = 293 and 333	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 140 and 580 g/l at 293 and 333 K, respectively. The authors did not specify whether the values were per liter of solvent or per liter of saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by adding (0.50 ± 0.1) g amounts of the powdered solute to (100 ± 1) ml of solvent until a saturated solution was obtained. The mass of the powder was recorded.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Poole, England, UK, no purification details were provided.
(2) Purity not given, Sigma-Aldrich, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
Solubility: ±5 g/l (estimated by compiler assuming solute added in increments of 0.50 g).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Ethanol; C_2H_6O; [64-17-5]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9145	0.0855

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) 99.6%, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Ethanol; C_2H_6O; [64-17-5]	[69]C. M. McLoughlin, W. A. M. McMinn, and T. R. A. Magee, Powder Technol. **134**, 40 (2003).
Variables:	**Prepared by:**
T/K = 293 and 333	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 240 and 720 g/l at 293 and 333 K, respectively. The authors did not specify whether the values were per liter of solvent or per liter of saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by adding (0.50 ± 0.1) g amounts of the powdered solute to (100 ± 1) ml of solvent until a saturated solution was obtained. The mass of the powder was recorded.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Poole, England, UK, no purification details were provided.
(2) Purity not given, Sigma-Aldrich, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
Solubility: ±5 g/l (estimated by compiler assuming solute added in increments of 0.50 g).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Ethanol; C_2H_6O; [64-17-5]	[92]G. D. Maia and M. Giulietti, J. Chem. Eng. Data **53**, 256 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
276.2	0.975	0.025
291.9	0.951	0.049
302.4	0.929	0.071
310.0	0.907	0.093
316.5	0.887	0.113
321.5	0.867	0.133
325.9	0.848	0.152
330.4	0.830	0.170
333.4	0.813	0.187
336.6	0.796	0.204

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating thermostated water bath, analytical balance, and drying oven.
Known amounts of solute and solvent were placed in the equilibrium vessel which was connected to the thermostated water bath. The vessel was agitated at 750 rpm as temperature was increased and decreased. By regulating the bath temperature, the authors were able to determine the temperature at which complete dissolution occurred (heating mode) and the temperature at which the first crystals formed (cooling mode).

Source and Purity of Chemicals:
(1) 99.5%, Anidrol Quimica, Diadema, Brazil, no purification details were given.
(2) 99.5%, Synthon Chemicals, no purification details were given.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Ethanol; C_2H_6O; [64-17-5]	[93]C. Lindenberg, M. Krättli, J. Cornel, M. Mazzotti, and J. Brozio, Cryst. Growth Des. **9**, 1124 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298	0.9427	0.0573
308	0.9118	0.0882
323	0.8578	0.1422

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute determined by *in situ* ATR-FTIR spectroscopic method. Experimental data are reported as grams of solute per kilogram of solvent. Mole fraction solubilities calculated by the compiler.

T/K	x_2[a]	x_1[b]
298	0.9425	0.0575
308	0.9124	0.0876
323	0.8549	0.1451

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute determined by a gravimetric method of analysis. Experimental data are reported as grams of solute per kilogram of solvent. Mole fraction solubilities calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed glass equilibrium cell equipped with a four-blade glass impeller and including blades, temperature controlling system, and an attenuated total reflectance-Fourier transform infrared (ATR-FTIR) probe.
Very little experimental details are given. Excess solute and solvent were placed in the equilibrium cell. The concentration of the dissolved solute was determined by ATR-FTIR spectroscopic methods. Solubilities were also determined by a gravimetric method.

Source and Purity of Chemicals:
(1) 99+%, Sigma-Aldrich, Switzerland, no purification details were given.
(2) 99.9%, Merck KGaA, Germany, no purification details were given.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Propanol; C_3H_8O; [71-23-8]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9502	0.04976

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Propanol; C_3H_8O; [71-23-8]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9582	0.0418

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) HPLC grade, Aldrich Chemical Company, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Propanol; C_3H_8O; [67-63-0]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9477	0.05232

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Propanol; C_3H_8O; [67-63-0]	[92]G. D. Maia and M. Giulietti, J. Chem. Eng. Data **53**, 256 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
281.6	0.987	0.013
291.8	0.968	0.032
304.1	0.937	0.063
312.9	0.909	0.091
316.1	0.898	0.102
320.4	0.882	0.118
322.7	0.872	0.128
325.8	0.857	0.143
327.7	0.847	0.153
330.2	0.833	0.167

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating thermostated water bath, analytical balance, and drying oven.
Known amounts of solute and solvent were placed in the equilibrium vessel which was connected to the thermostated water bath. The vessel was agitated at 750 rpm as temperature was increased and decreased. By regulating the bath temperature, the authors were able to determine the temperature at which complete dissolution occurred (heating mode) and the temperature at which the first crystals formed (cooling mode).

Source and Purity of Chemicals:
(1) 99.5%, Anidrol Quimica, Diadema, Brazil, no purification details were given.
(2) 99.9%, Synthon Chemicals, no purification details were given.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9538	0.04616

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9547	0.0453

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]

Original Measurements:
[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9464	0.05360

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

Original Measurements:
[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9681	0.03186

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [78-83-1]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9316	0.06844

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	Original Measurements:
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9603	0.03966

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9605	0.0395

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Aldrich Chemical Company, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9565	0.04345

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9656	0.03444

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9619	0.03812

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9182	0.08176

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9603	0.03973

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9607	0.0393

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9679	0.03205

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9607	0.03931

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9611	0.03892

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Heptanol; $C_7H_{16}O$; [111-37-3]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9614	0.0386

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:

(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Sigma Chemical Company, USA, no purification details were provided.

Estimated Error:

Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9642	0.03581

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9659	0.0341

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:

(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, Sigma Chemical Company, USA, no purification details were provided.

Estimated Error:

Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[94]S. L. Cassidy, P. A. Lympany, and J. A. Henry, J. Pharm. Pharmacol. **40**, 130 (1988).
Variables:	**Prepared by:**
T/K = 310	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 42.6 g/l of saturated solution, which corresponds to a solubility of $c_1 = 0.24 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Saturated solution was prepared at 310 K, and the concentration of the dissolved solute determined spectrophotometrically by reference to an absorbance curve obtained from absorbance measurements of standard solutions of known concentration.

Source and Purity of Chemicals:
(1) 98% to 100%, Eli Lilly Drug Company, USA, used as received. The authors studied the solubility of several drugs, and their only statement regarding purity was that all drugs were used as supplied at a purity of 90%–100%.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9697	0.03033

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9635	0.03652

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 3,7-Dimethyl-1-octanol; $C_{10}H_{22}O$; [106-21-8]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9696	0.03039

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[92]G. D. Maia and M. Giulietti, J. Chem. Eng. Data **53**, 256 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.7	0.983	0.017
301.1	0.975	0.025
305.1	0.967	0.033
308.2	0.959	0.041
313.6	0.944	0.056
318.3	0.929	0.071
323.7	0.908	0.092
327.9	0.888	0.112
330.6	0.874	0.126
333.9	0.855	0.145

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating thermostated water bath, analytical balance, and drying oven.
Known amounts of solute and solvent were placed in the equilibrium vessel which was connected to the thermostated water bath. The vessel was agitated at 750 rpm as temperature was increased and decreased. By regulating the bath temperature, the authors were able to determine the temperature at which complete dissolution occurred (heating mode) and the temperature at which the first crystals formed (cooling mode).

Source and Purity of Chemicals:
(1) 99.5%, Anidrol Quimica, Diadema, Brazil, no purification details were given.
(2) 99.9%, Synthon Chemicals, no purification details were given.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

3.7. 2-Acetoxybenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Propanone; C_3H_6O; [67-64-1]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9172	0.0828

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.
(2) Analytical Reagent grade, SDS, Peypin, France, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Propanone; C_3H_6O; [67-64-1]	[69]C. M. McLoughlin, W. A. M. McMinn, and T. R. A. Magee, Powder Technol. **134**, 40 (2003).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 250 g/l. The authors did not specify whether the value was per liter of solvent or per liter of saturated solution.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by adding (0.50 ± 0.1) g amounts of the powdered solute to (100 ± 1) ml of solvent until a saturated solution was obtained. The mass of the powder was recorded.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Poole, England, UK, no purification details were provided.
(2) Purity not given, Sigma-Aldrich, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
Solubility: ±5 g/l (estimated by compiler assuming solute added in increments of 0.50 g).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Propanone; C_3H_6O; [67-64-1]	[91]G. D. Maia and M. Giulietti, J. Chem. Eng. Data **53**, 256 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
281.9	0.939	0.061
290.6	0.925	0.075
297.9	0.912	0.088
304.4	0.899	0.101
310.6	0.886	0.114
315.3	0.873	0.127
319.8	0.861	0.139
323.3	0.849	0.151
326.3	0.838	0.162

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating thermostated water bath, analytical balance, and drying oven. Known amounts of solute and solvent were placed in the equilibrium vessel which was connected to the thermostated water bath. The vessel was agitated at 750 rpm as temperature was increased and decreased. By regulating the bath temperature, the authors were able to determine the temperature at which complete dissolution occurred (heating mode) and the temperature at which the first crystals formed (cooling mode).

Source and Purity of Chemicals:
(1) 99.5%, Anidrol Quimica, Diadema, Brazil, no purification details were given.
(2) 99.9%, Synthon Chemicals, no purification details were given.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

3.8. 2-Acetoxybenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[12]A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **32**, 1087 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9687	0.03133

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Acetoxybenzoic acid; $C_9H_8O_4$; [50-78-2] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[53]G. L. Perlovich and A. Bauer-Brandl, Pharm. Res. **20**, 471 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9815	0.0185

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:

(1) Analytical Reagent grade, Norsk Medisinaldepot, Oslo, Norway, no purification details were provided.

(2) HPLC grade, Merck Chemicals, Germany, no purification details were provided.

Estimated Error:

Temperature: ±0.01 K.

x_1: ±2.5% (relative error).

4. Solubility of 4-Acetoxybenzoic Acid in Organic Solvents

4.1. Critical evaluation of experimental solubility data

There is only a single published study regarding the solubility behavior of 4-acetoxybenzoic acid in organic solvents. Wang and Zhang[97] measured the mole fraction solubilities in ethanol as a function of temperature using a static and dynamic method. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 10, along with the MRD calculated according to Eq. (24). Examination of the numerical entries in the last column of Table 10 reveals that the static experimental method yielded the more consistent experimental values. Readers are reminded that Eq. (8) can only check data points for internal consistency with respect to temperature. The fact that one can accurately describe the experimental data does not mean that the data are accurate. In the case of the 4-acetoxybenzoic acid solubility data, there is a noticeable difference between the two experimental methods. The relative difference can be fairly large at times. For example the static method gave a mole fraction solubility of $x_1 = 0.002489$ for 4-acetoxybenzoic acid dissolved in ethanol at 298.15 K, versus a value of $x_1 = 0.002193$ determined with the dynamic method. The calculated relative difference between the two reported values is more than 10%.

TABLE 10. Parameters of the Modified Apelblat equation for describing the solubility of 4-acetoxybenzoic acid in ethanol[a]

Solvent	A	B	C	MRD (%)
Ethanol (dynamic method)	24.84	−4110	−1.781	5.599
Ethanol (static method)	−26.18	−1737	5.776	0.674

[a]Values of the coefficients and the mean relative deviations were taken from Wang and Zhang.[97]

The experimental solubility data for 4-acetoxybenzoic acid in ethanol are in Sec. 4.2.

4.2. 4-Acetoxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Acetoxybenzoic acid; $C_9H_8O_4$; [2345-34-8] (2) Ethanol; C_2H_6O; [64-17-5]	[97]H. Wang and W. Zhang, J. Chem. Eng. Data **54**, 1942 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9751	0.02489
303.2	0.9698	0.03018
308.2	0.9642	0.03584
313.2	0.9569	0.04315
318.2	0.9478	0.05217

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.
[c]Solubility determined by the static method.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9781	0.02193
303.2	0.9685	0.03149
308.2	0.9612	0.03876
313.2	0.9549	0.04514
318.2	0.9488	0.05117

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.
[c]Solubility determined by the dynamic method.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water-jacketed glass vessel, thermometer, analytical balance, laser monitoring system.
Solubilities were determined using both a static and dynamic method. In the static method, excess solute and solvent were placed in a water-jacketed vessel allowed to equilibrate with stirring for three days at constant temperature. Samples of the saturated liquid phase were decanted into Petri dishes of known mass and weighed. The samples were then evaporated to dryness and the solubility determined from the mass of the solid residue and the mass of the sample analyzed. In the dynamic solid method, an excess of carboxylic acid was added to a known mass of ethanol. The resulting suspension was stirred in a water-jacketed vessel for 1 h at constant temperature. A known mass of ethanol to the vessel through a buret until the solute completely dissolved. The dissolution was monitored with a laser monitoring system. When the last portion of solid solute disappeared, the penetrated light intensity reached its maximum value. The mass of the added solvent was recorded. The solubility of the carboxylic acid was calculated from the known masses of solute and ethanol.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, Milwaukee, WI, USA, no purification details provided.
(2) 99.55%, Tianjin Kewei Chemical Reagent, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: Authors report that the uncertainty in the solubility values is estimated to be ±0.5%. The differences between the experimental values based on the static and dynamic solubility methods are considerably larger, and more on the order of ±5% to 10% (relative error).

5. Solubility of 4-Acetylbenzoic Acid in Organic Solvents

5.1. Critical evaluation of experimental solubility data

Only a single published paper was found in the chemical and engineering literature regarding the solubility of 4-acetylbenzoic acid in organic solvents. Sunsandee *et al.*[98] measured the solubility of 4-acetylbenzoic acid in 1-methyl-4-(1-methylethyl)benzene (also called *p*-cymene), *tert*-butylbenzene, and ethanoic acid from 303 to 473 K. The authors described the observed solubility data in terms of both the Modified Apelblat model [Eq. (8)] and Buchowski λh-model [Eq. (9)]. The calculated curve-fit equation coefficients and squared correlation coefficients are given in Tables 11 and 12 for the Modified Apelblat and Buchowski λh-models, respectively. The experimental solubility data are internally consistent as evidenced by the near unity values of the squared correlation coefficients.

The experimental solubility data for 4-acetylbenzoic acid in organic solvents are given in Secs. 5.2 and 5.3.

TABLE 11. Parameters of the Modified Apelblat equation for describing the solubility of 4-acetylbenzoic acid in various organic solvents

Solvent	T/K	A	B	C	R^2
p-Cymene[a]	303–453	−125.42	3239.20	18.99	0.9990
tert-Butylbenzene[a]	303–453	−116.93	2858.70	17.73	0.9990
Ethanoic acid[a]	303–453	−114.80	3288.30	17.12	0.9980

[a] Values of the coefficients and squared correlation coefficients were taken from Sunsandee *et al.*[98]

TABLE 12. Parameters of the Buchowski λh equation for describing the solubility of 4-acetylbenzoic acid in various organic solvents

Solvent	T/K	λ	h	R^2
p-Cymene[a]	303–453	0.045739	47820.72	0.9980
tert-Butylbenzene[a]	303–453	0.042173	42168.65	0.9990
Ethanoic acid[a]	303–453	0.036581	70114.79	0.9990

[a] Values of the coefficients and squared correlation coefficients were taken from Sunsandee *et al.*[98]

5.2. 4-Acetylbenzoic acid solubility data in aromatic hydrocarbons

Components: (1) 4-Acetylbenzoic acid; $C_9H_7O_3$; [586-89-0] (2) 1-Methyl-4-(1-methylethyl) benzene; $C_{10}H_{14}$; [99-87-6]	**Original Measurements:** [98] N. Sunsandee, M. Hronec, M. Stolcova, N. Leepipatpiboon, and U. Pancharoen, J. Mol. Liq. **180**, 252 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.15	0.9980	0.00199
313.15	0.9974	0.00260
323.15	0.9965	0.00346
333.15	0.9955	0.00451
343.15	0.9940	0.00602
353.15	0.9920	0.00802
363.15	0.9895	0.01050
373.15	0.9860	0.01398
383.15	0.9817	0.01828
393.15	0.9758	0.02417
403.15	0.9687	0.03134
413.15	0.9589	0.04114
423.15	0.9459	0.05413
433.15	0.9295	0.07046
443.15	0.9080	0.09202
453.15	0.8794	0.12063

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Stainless steel closed equilibrium vessel equipped with magnetic stirrer, analytical balance, high-performance liquid chromatographic system, thermostated silicone oil bath, and digital density meter.
Excess solute and solvent were allowed to equilibrate with stirring in a thermostated silicone oil bath for 90 min. The stirring was suspended and the suspended particles were allowed to settle to the bottom of the vessel for 120 min. An aliquot of the saturated solution was withdrawn, transferred to a tared volumetric flask, and then weighed to determine the amount of sample withdrawn. The concentration of the dissolved solute was determined by high-performance liquid chromatographic analysis. The density of the saturated was also measured to allow the measured solubilities in units of molarity to be converted to mole fraction solubilities.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, was used as received.
(2) 99.9% (by HPLC analysis), Sigma-Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Acetylbenzoic acid; $C_9H_7O_3$; [586-89-0] (2) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6]	[98]N. Sunsandee, M. Hronec, M. Stolcova, N. Leepipatpiboon, and U. Pancharoen, J. Mol. Liq. **180**, 252 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.15	0.9979	0.00205
313.15	0.9973	0.00271
323.15	0.9964	0.00357
333.15	0.9953	0.00473
343.15	0.9938	0.00618
353.15	0.9918	0.00817
363.15	0.9894	0.01063
373.15	0.9862	0.01384
383.15	0.9818	0.01822
393.15	0.9761	0.02387
403.15	0.9690	0.03098
413.15	0.9600	0.03999
423.15	0.9480	0.05198
433.15	0.9321	0.06785
443.15	0.9123	0.08767
453.15	0.8860	0.11403

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Stainless steel closed equilibrium vessel equipped with magnetic stirrer, analytical balance, high-performance liquid chromatographic system, thermostated silicone oil bath, and digital density meter.
Excess solute and solvent were allowed to equilibrate with stirring in a thermostated silicone oil bath for 90 min. The stirring was suspended and the suspended particles were allowed to settle to the bottom of the vessel for 120 min. An aliquot of the saturated solution was withdrawn, transferred to a tared volumetric flask, and then weighed to determine the amount of sample withdrawn. The concentration of the dissolved solute was determined by high-performance liquid chromatographic analysis. The density of the saturated was also measured to allow the measured solubilities in units of molarity to be converted to mole fraction solubilities.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, was used as received.
(2) 99.9% (by HPLC analysis), Sigma-Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error, estimated by compiler).

5.3. 4-Acetylbenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Acetylbenzoic acid; $C_9H_7O_3$; [586-89-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[98]N. Sunsandee, M. Hronec, M. Stolcova, N. Leepipatpiboon, and U. Pancharoen, J. Mol. Liq. **180**, 252 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.15	0.9978	0.00218
313.15	0.9973	0.00269
323.15	0.9967	0.00332
333.15	0.9958	0.00416
343.15	0.9948	0.00515
353.15	0.9936	0.00644
363.15	0.9919	0.00807
373.15	0.9899	0.01005
383.15	0.9875	0.01253
393.15	0.9843	0.01567
403.15	0.9805	0.01953
413.15	0.9755	0.02453
423.15	0.9695	0.03047
433.15	0.9610	0.03896
443.15	0.9527	0.04731
453.15	0.9417	0.05833

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Stainless steel closed equilibrium vessel equipped with magnetic stirrer, analytical balance, high-performance liquid chromatographic system, thermostated silicone oil bath, and digital density meter.
Excess solute and solvent were allowed to equilibrate with stirring in a thermostated silicone oil bath for 90 min. The stirring was suspended and the suspended particles were allowed to settle to the bottom of the vessel for 120 min. An aliquot of the saturated solution was withdrawn, transferred to a tared volumetric flask, and then weighed to determine the amount of sample withdrawn. The concentration of the dissolved solute was determined by high-performance liquid chromatographic analysis. The density of the saturated was also measured to allow the measured solubilities in units of molarity to be converted to mole fraction solubilities.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, was used as received.
(2) 99.8% (by HPLC analysis), Sigma-Aldrich Chemical Company, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error, estimated by compiler).

6. Solubility of 2-Aminobenzoic Acid in Organic Solvents

6.1. Critical evaluation of experimental solubility data

Only two published papers were found in the chemical and engineering literature regarding the solubility of 2-aminobenzoic acid in organic solvents. Jia *et al.*[99] determined the solubility of 2-aminobenzoic acid in 1-octanol in the temperature range of 293–323 K. The calculated curve-fit parameters from the Buchowski λh-model [Eq. (9)] of $\lambda = 0.4895$ and $h = 4520.42$ described the observed solubility data to within a mean relative deviation of 0.9%.

Lazzell and Johnston[100] measured the solubility of 2-aminobenzoic acid in benzene, ethyl ethanoate, trichloromethane, methanol, ethanol, and 1-butanol as a function of temperature. Except for 1-butanol, the measurements went from 298 K to well above the normal boiling temperature of the solvent. The internal consistency of the benzene, trichloromethane, and ethanol datasets was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model to yield the following representations:

$$\ln x_1(\text{in benzene}) = -92.104 + \frac{113.71}{T} + 15.248 \ln T, \quad (27)$$

$$\ln x_1(\text{in trichloromethane}) = -80.747 + \frac{113.94}{T} + 13.370 \ln T, \quad (28)$$

$$\ln x_1(\text{in ethanol}) = -48.945 + \frac{114.60}{T} + 8.074 \ln T. \quad (29)$$

There were too few data points in the ethyl ethanoate, methanol, and 1-butanol datasets to perform a meaningful regression analysis. The average absolute deviations between the observed experimental data and back-calculated values based on Eqs. (27)–(29) (of 5.36%, 3.61%, and 0.62%, respectively) are quite small given the range of mole fraction solubilities covered by each of the three datasets. In the case of benzene, the observed solubilities ranged from $x_1 = 0.0081$ to $x_1 = 0.8064$. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 2-aminobenzoic acid in organic solvents are given in Secs. 6.2–6.5.

6.2. 2-Aminobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Aminobenzoic acid; $C_7H_7NO_2$; [118-92-3] (2) Benzene; C_6H_6; [71-43-2]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9919	0.0081
348.9	0.9129	0.0871
362.7	0.8687	0.1313
366.5	0.8364	0.1636
374.8	0.7778	0.2222
381.5	0.7074	0.2926
383.5	0.6504	0.3496
392.8	0.4912	0.5088
392.5	0.4897	0.5103
398.3	0.3826	0.6174
399.5	0.3531	0.6469
403.1	0.2874	0.7126
408.4	0.1936	0.8064

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:

(1) Certified Pure, Chemical source not given, was recrystallized several times from hot water, then from chloroform to give a sample having a melting point of 419.3 K.

(2) Thiophene-free, Chemical source not given, was dried over sodium and distilled before use.

Estimated Error:

Temperature: Not given in paper.

x_1: ±5% (relative error, estimated by compiler).

6.3. 2-Aminobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 2-Aminobenzoic acid; $C_7H_7NO_2$; [118-92-3] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.8529	0.1471
350.0	0.7027	0.2973
381.2	0.4718	0.5282
394.0	0.3497	0.6503

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot water, then from chloroform to give a sample having a melting point of 419.3 K.
(2) USP grade, Chemical source not given, washed several times with aqueous sodium carbonate, and then with water until the aqueous layer was neutral. The sample was further purified by drying over calcium chloride and then distilling two times before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

6.4. 2-Aminobenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Aminobenzoic acid; $C_7H_7NO_2$; [118-92-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9843	0.0157
349.7	0.8876	0.1124
362.1	0.8117	0.1883
373.6	0.7093	0.2907
384.0	0.5686	0.4314

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot water, then from chloroform to give a sample having a melting point of 419.3 K.
(2) Certified Pure, Chemical source not given, was dried over calcium chloride and distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

6.5. 2-Aminobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2-Aminobenzoic acid; $C_7H_7NO_2$; [118-92-3] (2) Methanol; CH_4O; [67-56-1]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9238	0.0762
323.9	0.8630	0.1370
350.3	0.7408	0.2592

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot water, then from chloroform to give a sample having a melting point of 419.3 K.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Aminobenzoic acid; $C_7H_7NO_2$; [118-92-3] (2) Ethanol; C_2H_6O; [64-17-5]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9225	0.0775
341.1	0.7781	0.2219
350.5	0.7306	0.2694
359.7	0.6697	0.3303
367.1	0.6181	0.3819
398.7	0.2608	0.7392

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot water, then from chloroform to give a sample having a melting point of 419.3 K.
(2) 95%, Chemical source not given, was refluxed with lime and distilled. The sample was further purified by drying over sodium and distilling twice before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Aminobenzoic acid; $C_7H_7NO_2$; [118-92-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
353.3	0.7320	0.2680
377.8	0.5514	0.4486

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot water, then from chloroform to give a sample having a melting point of 419.3 K.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Aminobenzoic acid; $C_7H_7NO_2$; [118-92-3] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[99]Q. Jia, P. Ma, S. Ma, and C. Wang, Chin. J. Chem. Eng. **15**, 710 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.30	0.9444	0.05555
298.45	0.9384	0.06159
299.95	0.9352	0.06478
301.80	0.9318	0.06817
303.15	0.9288	0.07116
305.05	0.9214	0.07512
307.05	0.9214	0.07856
308.55	0.9185	0.08146
309.65	0.9161	0.08392
311.35	0.9124	0.08761
313.35	0.9081	0.09187
315.95	0.9026	0.09735
317.75	0.8987	0.1013
320.15	0.8924	0.1076
322.25	0.8891	0.1109

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature circulating bath, stirrer, analytical balance, and laser monitoring system.
Solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent were placed in a stoppered equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and the temperature slowly increased until all of the solid dissolved. Near the dissolution temperature, the temperature was increased at a rate of 0.2 K per 20 min. Complete dissolution was determined using a laser monitoring system.

Source and Purity of Chemicals:
(1) 99+%, Chemical source not specified, no purification details were provided.
(2) 99+%, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

7. Solubility of 3-Aminobenzoic Acid in Organic Solvents

7.1. Critical evaluation of experimental solubility data

The have been only three published studies involving the solubility of 3-aminobenzoic acid in organic solvents. Hancock *et al.*[54] measured the solubility of 3-aminobenzoic acid in cyclohexane and benzene at 303 K based on a gravimetric method. Svärd *et al.*[101] determined the solubility of two polymorphic forms of 3-aminobenzoic acid in ethyl ethanoate, methanol, and ethanenitrile using a gravimetric method. Differential scanning calorimetry showed both polymorphs melting without any prior solid–solid transformations, with measured enthalpies of fusion and melting temperatures of $\Delta H_1^{\text{fus}} = 35.51$ kJ mol^{-1} and $T_{\text{mp}} = 445.2$ K, and $\Delta H_1^{\text{fus}} = 26.74$ kJ mol^{-1} and $T_{\text{mp}} = 451.2$ K for the forms I and II, respectively. Form I was characterized by dendritic growth, forming small cascades of threads, possibly due to twinning. Form II, on the other hand, developed into needle-like crystals that can be grown to several millimeters in length. Form II was the more soluble of the two polymorphs as one might expect from its lower enthalpy of fusion. The authors fit the solubility data for each solvent and each polymorph to Eq. (22). The calculated equation coefficients (A, B, and C) are given in Table 13, along with the χ^2 "goodness-of-fit" calculated by the Origin 6.1 statistical software. Graphs of the mole fraction solubility versus temperature given in the paper fell on smooth curves, and did not indicate any obvious outlier data points.

Lazzell and Johnston[100] measured the solubility of 3-aminobenzoic acid in benzene, ethyl ethanoate, trichloromethane, methanol, ethanol, and 1-butanol as a function of temperature. Except for 1-butanol, the measurements went from 298 K to well above the normal boiling temperature of the solvent. The internal consistency of the benzene and ethanol datasets was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model to yield the following representations:

$$\ln x_1(\text{in benzene}) = -255.914 + \frac{110.95}{T} + 41.973 \ln T, \quad (30)$$

$$\ln x_1(\text{in ethanol}) = -65.997 + \frac{114.72}{T} + 10.772 \ln T. \quad (31)$$

The experimental value at 298 K had to be removed from the benzene dataset in order to obtain a reasonable correlation equation. There were too few data points in the ethyl ethanoate, trichloromethane, methanol, and 1-butanol datasets to perform a meaningful regression analysis. The average absolute deviations between the observed experimental data and back-calculated values based on Eqs. (30) and (31) of 18.36% and 7.88% are larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0423$ to $x_1 = 0.6704$ for benzene and $x_1 = 0.0152$ to $x_1 = 0.7806$ for ethanol. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 3-aminobenzoic acid in organic solvents are given in Secs. 7.2–7.6.

TABLE 13. Parameters of Eq. (22) describing the solubility of 3-aminobenzoic acid in ethyl ethanoate, ethanenitrile, and methanol[a]

Solvent	A	B	C	χ^2
Ethyl ethanoate (Form I)	−31.57	2471.76	0.06134	0.00048
Ethyl ethanoate (Form II)	−8.55	−242.26	0.01841	0.00014
Methanol (Form I)	−11.93	−279.14	0.02891	0.00031
Ethanenitrile (Form I)	−36.07	2604.92	0.07192	0.00187
Ethanenitrile (Form II)	16.47	−4464.59	−0.02117	0.00009

[a] Values of the coefficients and goodness-of-fit were taken from Svärd *et al.*[101]

7.2. 3-Aminobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000275

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

7.3. 3-Aminobenzoic acid solubility data in aromatic hydrocarbons

Components:	Original Measurements:
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000771

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

Components:	Original Measurements:
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Benzene; C_6H_6; [71-43-2]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9992	0.0008
407.6	0.9577	0.0423
411.7	0.9447	0.0553
416.9	0.9246	0.0754
423.6	0.8740	0.1260
426.7	0.8046	0.1954
429.9	0.6508	0.3492
434.9	0.3296	0.6704

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, was recrystallized several times from hot water, then from 95% ethanol, and finally from boiling water. The purified sample had a melting point temperature of 451.1 K.
(2) Thiophene-free, Chemical Source not given, was dried over sodium and distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

7.4. 3-Aminobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[101]M. Svärd, F. L. Nordström, and A. C. Rasmuson, Cryst. Growth Des. **10**, 195 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9957	0.00429
288.2	0.9951	0.00490
293.3	0.9944	0.00561
298.2	0.9933	0.00670
303.2	0.9917	0.00830
308.2	0.9903	0.00972
313.2	0.9883	0.01170
318.2	0.9864	0.01362
323.2	0.9835	0.01654

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for polymorph form I. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Experimental Values

T/K	x_2[a]	x_1[b]
273.2	0.9877	0.01227
278.2	0.9866	0.01338
283.2	0.9848	0.01522
288.2	0.9832	0.01675
293.3	0.9813	0.01867
298.2	0.9789	0.02106
303.2	0.9771	0.02293

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for polymorph form II. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8%, HiperSolv, VWR Scientific, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9870	0.0130
383.7	0.8824	0.1176
418.3	0.5281	0.4719

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, was recrystallized several times from hot water, then from 95% ethanol, and finally from boiling water. The purified sample had a melting point temperature of 451.1 K.
(2) USP grade, Chemical source not given, washed several times with aqueous sodium carbonate, and then with water until the aqueous layer was neutral. The sample was further purified by drying over calcium chloride and then distilling two times before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

7.5. 3-Aminobenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9995	0.0005
398.0	0.9635	0.0365
406.1	0.9437	0.0563
425.9	0.6787	0.3213

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, was recrystallized several times from hot water, then from 95% ethanol, and finally from boiling water. The purified sample had a melting point temperature of 451.1 K.
(2) Certified Pure, Chemical source not given, was dried over calcium chloride and distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

7.6. 3-Aminobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Methanol; CH_4O; [67-56-1]	[101]M. Svärd, F. L. Nordström, and A. C. Rasmuson, Cryst. Growth Des. **10**, 195 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9911	0.00893
288.2	0.9897	0.01025
293.3	0.9881	0.01194
298.2	0.9860	0.01399
303.2	0.9831	0.01691
308.2	0.9798	0.02016
313.2	0.9771	0.02294
318.2	0.9731	0.02686
323.2	0.9686	0.03135

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for polymorph form I. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Sigma-Aldrich Chemical Company, USA, used as received.
(2) 99.9+%, VWR Scientific, USA, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

Components:
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9830	0.0170
359.4	0.9027	0.0973
382.8	0.7993	0.2007

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, was recrystallized several times from hot water, then from 95% ethanol, and finally from boiling water. The purified sample had a melting point temperature of 451.1 K.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9848	0.0152
371.8	0.8811	0.1189
388.7	0.7589	0.2411
413.7	0.5208	0.4792
436.8	0.2194	0.7806

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, was recrystallized several times from hot water, then from 95% ethanol, and finally from boiling water. The purified sample had a melting point temperature of 451.1 K.
(2) 95%, Chemical source not given, was refluxed with lime and distilled. The sample was further purified by drying over sodium and distilling twice before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
400.4	0.7928	0.2072
411.9	0.7065	0.2935

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Certified Pure, was recrystallized several times from hot water, then from 95% ethanol, and finally from boiling water. The purified sample had a melting point temperature of 451.1 K.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

7.7. 3-Aminobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3-Aminobenzoic acid; $C_7H_7NO_2$; [99-05-8] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[101]M. Svärd, F. L. Nordström, and A. C. Rasmuson, Cryst. Growth Des. **10**, 195 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9984	0.00157
288.2	0.9982	0.00177
293.3	0.9979	0.00214
298.2	0.9972	0.00282
303.2	0.9966	0.00337
308.2	0.9955	0.00447
313.2	0.9944	0.00561
318.2	0.9933	0.00673
323.2	0.9917	0.00830

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for polymorph form I. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9958	0.00423
288.2	0.9950	0.00501
293.3	0.9940	0.00603
298.2	0.9930	0.00695
303.2	0.9919	0.00813

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for polymorph form II. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8%, LiChrosolv, VWR Scientific, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

8. Solubility of 4-Aminobenzoic Acid in Organic Solvents

8.1. Critical evaluation of experimental solubility data

There have been several published studies[51,102–105] investigating the solubility behavior of 4-aminobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Daniels *et al.*[103] measured the solubility of 4-aminobenzoic acid in 13 alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 1-pentanol, 2-pentanol, 3-methyl-1-butanol, 1-hexanol, 1-heptanol, 1-octanol, and 1-decanol), and in one cyclic ether (1,4-dioxane) at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 4-aminobenzoic acid. The authors were able to assemble a total of 26 $\log_{10}$ (SR or P) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 4-aminobenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -1.37$.[106] The McGowan volume of 4-aminobenzoic acid, $V = 1.0315$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 1.075$. This left three solute descriptors (S, A, and B) still to be determined. The 26 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 1.650$, $A = 0.940$, and $B = 0.600$, that best described the $\log_{10}$ (SR or P) values. The calculated molecular solute descriptors reproduced the $\log_{10}$ (SR or P) values to within an average standard deviation of 0.120 $\log_{10}$ units.

TABLE 14. Comparison between observed and calculated molar solubilities of 4-aminobenzoic acid based on the Abraham model, Eq. (20)

Solvent	$\log_{10} c_1^{\text{exp}}$	$\log_{10} c_1^{\text{calc}}$; Eq. (20)
Ethanol	−0.082	−0.222
1-Propanol	−0.360	−0.410
2-Propanol	−0.384	−0.387
1-Butanol	−0.470	−0.593
2-Butanol	−0.520	−0.519
2-Methyl-1-propanol	−0.724	−0.675
1-Pentanol	−0.616	−0.652
2-Pentanol	−0.673	−0.682
3-Methyl-1-butanol	−0.742	−0.780
1-Hexanol	−0.670	−0.722
1-Heptanol	−0.792	−0.811
1-Octanol	−0.877	−0.814
1-Decanol	−1.040	−0.996
1,1′-Oxybisethane	−0.888[a]	−1.027
1,4-Dioxane	−0.096	−0.122
Propanone	−0.158[a]	−0.278

[a]Experimental data from a study by Barra *et al.*[102] All other experimental values are from Daniels *et al.*[103]

After the 4-aminobenzoic acid solubility study was published, Abraham model correlations have been developed for 3-methyl-1-butanol and 2-pentanol, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Table 1) will be used in illustrating the ability of the Abraham model to correlate the experimental 4-aminobenzoic acid solubility data. Table 14 compares the experimental $\log_{10} c_1$ values to calculated values based on Eq. (20) of the Abraham model.

For comparison purposes, the measured mole fraction solubilities of 4-aminobenzoic acid, x_1, determined by Daniels *et al.*[103] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\text{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\text{solvent}}]$). The molar volume of the hypothetical subcooled liquid 4-aminobenzoic acid is $V_{\text{solute}} = 106.49$ cm^3 mol^{-1}. Examination of the numerical entries in Table 14 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset. Included in Table 14 are experimental solubility measurements for 4-aminobenzoic acid dissolved in 1,1′-oxybisethane and propanone from the solubility study of Barra *et al.*[102]

Barra *et al.*[102] published solubility data for 4-aminobenzoic acid in two saturated hydrocarbons (heptane and cyclohexane), in one aromatic hydrocarbon (benzene), in one alkyl alkanoate (ethyl ethanoate), in one alkyl ether (1,1′-oxybisethane) and one cyclic ether (1,4-dioxane), in two chloroalkanes (trichloromethane and 1,2-dichloroethane) and one chloroaromatic hydrocarbon (chlorobenzene), in seven alcohols [methanol, ethanol, 1-pentanol, 1-octanol, 1,2-ethanediol, 1,2-propanediol, and 1,2,3-propanetriol (also referred to as glycerol)], in one alkanone (propanone) and one aromatic ketone (acetophenone), and in four miscellaneous organic solvents (ethanoic acid, propanoic acid, formamide, and *N*,*N*-dimethylformamide) at 298 K. Lin and Nash[51] determined 4-aminobenzoic acid solubilities at 298 K in 16 different organic solvents, including hexane, ethyl ethanoate, tetrahydrofuran, methanol, 1-propanol, 3-methyl-3-pentanol, 1,2-propanediol, 1,3-propanediol, butyl 2-hydroxypropanoate (also called butyl lactate), and 2-ethoxyethanol. Abraham model equation coefficients are available for several of the solvents studied by Barra *et al.*[102] and by Lin and Nash.[51] Several solvents were not included in the Table 13 comparison because of the likelihood of dimerization in the nonpolar alkane and aromatic hydrocarbon solvents, or concerns regarding the formation of possible solid solvates. The Abraham model requires that the solute exist in the same crystalline form in both water and the organic solvent. The measurements of Barra *et al.*[102] do provide independent experimental values for the solubility of 4-aminobenzoic acid in ethanol, 1-pentanol, 1-octanol, and 1,4-dioxane. The mole fraction solubilities reported by Barra *et al.*[102] are about 10% less than the published values of Daniels *et al.*,[103] namely, $x_1 = 0.0465$ versus $x_1 = 0.0506$ for ethanol, $x_1 = 0.0234$ versus $x_1 = 0.0263$ for 1-pentanol, $x_1 = 0.0181$ versus $x_1 = 0.0209$ for 1-octanol, and $x_1 = 0.0632$ versus $x_1 = 0.0700$ for 1,4-dioxane.

There are three or more experimental data points in a few solvents listed in Secs. 8.2–8.10 to compute recommended values. The recommended mole fraction solubilities of 4-aminobenzoic acid at 298 K are as follows: $x_1 = 0.0566$ for ethyl ethanoate [arithmetic average of $x_1 = 0.0576$,[102] 0.0532,[51] 0.0574,[104] and 0.0589 (Ref. 104)]; $x_1 = 0.0570$ for methanol [arithmetic average of $x_1 = 0.0539$,[102] 0.0576,[51] and 0.0594 (Ref. 100)]; and $x_1 = 0.192$ for 1-octanol [arithmetic average of $x_1 = 0.0187$,[99] 0.02088,[103] and 0.01806 (Ref. 102)].

Jia *et al.*[99] determined the solubility of 4-aminobenzoic acid in 1-octanol in the temperature range of 293–323 K. The calculated curve-fit parameters from the Buchowski λh-model [Eq. (9)] of $\lambda = 0.2257$ and $h = 9393.6$ described the observed solubility data to within a mean relative deviation of 0.9%.

Lazzell and Johnston[100] measured the solubility of 4-aminobenzoic acid in benzene, ethyl ethanoate, trichloromethane, methanol, ethanol, and 1-butanol as a function of temperature. Except for ethyl ethanoate and 1-butanol, the measurements went from 298 K to well above the normal boiling temperature of the solvent. The internal consistency of the benzene, ethyl ethanoate, and ethanol datasets was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model to yield the following representations:

$$\ln x_1(\text{in benzene}) = -185.559 + \frac{112.06}{T} + 30.304 \ln T, \tag{32}$$

$$\ln x_1(\text{in ethyl ethanoate}) = -54.622 + \frac{114.72}{T} + 8.884 \ln T, \tag{33}$$

$$\ln x_1(\text{in ethanol}) = -45.766 + \frac{114.89}{T} + 7.429 \ln T. \tag{34}$$

The experimental value at 298 K had to be removed from the benzene dataset in order to obtain a reasonable correlation equation. There were too few data points in the trichloromethane, methanol, and 1-butanol datasets to perform a meaningful regression analysis. The average absolute deviations between the observed experimental data and back-calculated values based on Eqs. (32)–(34) of 15.00%, 3.07%, and 4.29% are larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0211$ to $x_1 = 0.5342$ for benzene, $x_1 = 0.1219$ to $x_1 = 0.4840$ for ethyl ethanoate, and $x_1 = 0.0497$ to $x_1 = 0.6552$ for ethanol. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 4-aminobenzoic acid in the different organic solvents are in Secs. 8.2–8.10.

8.2. 4-Aminobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Hexane; C_6H_{14}; [110-54-3]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.000001

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Heptane; C_7H_{16}; [142-82-5]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000061

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000116

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.00000087

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±10.0% (relative error, estimated by compiler).

8.3. 4-Aminobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9996	0.000427

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±5% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Benzene; C_6H_6; [71-43-2]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9998	0.000210

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Benzene; C_6H_6; [71-43-2]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9996	0.0004
394.9	0.9789	0.0211
413.1	0.9502	0.0498
428.0	0.8586	0.1414
428.4	0.8434	0.1566
429.7	0.8176	0.1824
433.0	0.7150	0.2850
433.4	0.6763	0.3237
438.2	0.4658	0.5342

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot aqueous solution, then from 95% ethanol, and finally from hot water. The purified solute had a melting point temperature of 460.2 K.
(2) Thiophene-free, Chemical source not given, was dried over sodium and distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

8.4. 4-Aminobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9424	0.0576

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9468	0.0532

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[104]S. Gracin and A. C. Rasmuson, Cryst. Growth Des. **4**, 1013 (2004).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
268.2	0.9554	0.0446
273.2	0.9554	0.0446
278.2	0.9541	0.0459
283.2	0.9522	0.0478
288.2	0.9491	0.0509
293.2	0.9459	0.0541
297.2	0.9431	0.0569
301.2	0.9411	0.0589
305.2	0.9383	0.0617
309.2	0.9360	0.0640
315.2	0.9282	0.0718
323.2	0.9235	0.0765

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for polymorph α (needles). Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Experimental Values

T/K	x_2[a]	x_1[b]
262.2	0.9608	0.0392
268.2	0.9608	0.0392
273.2	0.9608	0.0392
278.2	0.9581	0.0419
283.2	0.9551	0.0449
288.2	0.9508	0.0492
293.2	0.9470	0.0530
297.2	0.9428	0.0572

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for polymorph form β (prisms). Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, oven, and a heating and refrigeration circulator.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in an oven. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8%, HiperSolv, VWR Scientific, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

Components:	Original Measurements:
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
355.3	0.8781	0.1219
385.3	0.7693	0.2307
404.4	0.6525	0.3475
409.8	0.5805	0.4195
417.2	0.5160	0.4840

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:

(1) Certified Pure, Chemical source not given, was recrystallized several times from hot aqueous solution, then from 95% ethanol, and finally from hot water. The purified solute had a melting point temperature of 460.2 K.

(2) USP grade, Chemical source not given, washed several times with aqueous sodium carbonate, and then with water until the aqueous layer was neutral. The sample was further purified by drying over calcium chloride and then distilling two times before use.

Estimated Error:

Temperature: Not given in paper.

x_1: ±5% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,2,3-Triacetoxypropane; $C_9H_{14}O_6$; [102-76-1]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9224	0.0776

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:

(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.

(2) Purity not given, Unichema International, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K (estimated by compiler).

x_1: ±3% (relative error, estimated by compiler).

8.5. 4-Aminobenzoic acid solubility data in ethers

Components:	Original Measurements:
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9864	0.0136

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.

(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3.0% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[105]P. K. Takayama, N. Nambu, and T. Nagai, Chem. Pharm. Bull. **25**, 879 (1977).
Variables:	**Prepared by:**
T/K = 283	W. E. Acree, Jr.

Experimental Values

The solubility was given graphically in the paper as a plot of molar concentration of the solute versus the concentration of ligand added. From the graph the compiler estimated a molar solubility of $c_1 = 0.102$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were sealed in vials and incubated for 48 h at 283 K. A 1 ml sample of the supernatant was withdrawn and the solvent evaporated at 323 K. The residue was dissolved in water or ethanol, and the concentration of the solute determined from spectroscopic absorbance measurements.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, was recrystallized from water before use.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: No information was given.

c_1: ±5% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.767	0.233

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.

Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.

(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:

Temperature: ±0.02 K.

x_1: ±1.0% (relative error).

Components:	Original Measurements:
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7830	0.2170

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, and high-performance liquid chromatograph.

Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:

(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.

(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K (estimated by compiler).

x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9300	0.06998

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9368	0.0632

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.922	0.078

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,2-Dimethoxyethane; $C_4H_{10}O_2$; [110-71-4]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7872	0.2128

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) Purity not given, Hoechst Chemikalien, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 2,5,8,11-Tetraoxadodecane; $C_8H_{18}O_4$; [112-49-2]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6435	0.3565

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

8.6. 4-Aminobenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9984	0.001558

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9987	0.0013
409.9	0.9475	0.0525
429.6	0.7010	0.2990

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot aqueous solution, then from 95% ethanol, and finally from hot water. The purified solute had a melting point temperature of 460.2 K.
(2) Certified Pure, Chemical source not given, was dried over calcium chloride and distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9971	0.00292

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9995	0.000485

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

8.7. 4-Aminobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Methanol; CH_4O; [67-56-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9461	0.0539

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Methanol; CH_4O; [67-56-1]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9424	0.0576

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Methanol; CH_4O; [67-56-1]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9406	0.0594
359.7	0.8225	0.1775
381.5	0.7313	0.2687

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:
(1) Certified Pure, Chemical source not given, was recrystallized several times from hot aqueous solution, then from 95% ethanol, and finally from hot water. The purified solute had a melting point temperature of 460.2 K.
(2) Purity not given, Chemical source not given, purification details were not provided.

Estimated Error:
Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethanol; C_2H_6O; [64-17-5]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9494	0.05062

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethanol; C_2H_6O; [64-17-5]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9535	0.0465

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethanol; C_2H_6O; [64-17-5]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9503	0.0497
349.0	0.8644	0.1356
354.5	0.8471	0.1529
361.9	0.7996	0.2004
372.2	0.7796	0.2204
388.2	0.7000	0.3000
413.3	0.5199	0.4801
428.4	0.3448	0.6552

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:

(1) Certified Pure, Chemical source not given, was recrystallized several times from hot aqueous solution, then from 95% ethanol, and finally from hot water. The purified solute had a melting point temperature of 460.2 K.
(2) 95%, Chemical source not given, was refluxed with lime and distilled. The sample was further purified by drying over sodium and distilling twice before use.

Estimated Error:

Temperature: Not given in paper.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9668	0.03316

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9671	0.0329

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:

(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 2-Propanol; C_3H_8O; [67-63-0]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9678	0.03218

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9686	0.03139

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[100]C. L. Lazzell and J. Johnston, J. Phys. Chem. **32**, 1331 (1928).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
407.7	0.6664	0.3336
426.4	0.4490	0.5510

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a solution of sodium hydroxide standardized against the pure acid.

Source and Purity of Chemicals:

(1) Certified Pure, Chemical source not given, was recrystallized several times from hot aqueous solution, then from 95% ethanol, and finally from hot water. The purified solute had a melting point temperature of 460.2 K.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: Not given in paper.

x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9719	0.02808

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9825	0.01751

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9737	0.02630

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9766	0.02338

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.

(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9767	0.02325

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9801	0.01989

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9734	0.02664

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 3-Methyl-3-pentanol; $C_6H_{14}O$; [77-74-3]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9639	0.0361

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, and high-performance liquid chromatograph.

Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:

(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.

(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K (estimated by compiler).

x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9772	0.02277

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9791	0.02088

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9819	0.01806

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.

(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[99]Q. Jia, P. Ma, S. Ma, and C. Wang, Chin. J. Chem. Eng. **15**, 710 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.95	0.9815	0.01849
300.85	0.9798	0.02076
303.55	0.9781	0.02186
303.45	0.9774	0.02257
305.80	0.9769	0.02307
307.65	0.9751	0.02493
308.85	0.9745	0.02550
309.90	0.9739	0.02605
310.85	0.9734	0.02659
311.75	0.9729	0.02710
313.35	0.9719	0.02814
315.15	0.9707	0.02926
318.35	0.9683	0.03165
320.05	0.9672	0.03276

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature circulating bath, stirrer, analytical balance, and laser monitoring system.

Solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent were placed in a stoppered equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and the temperature slowly increased until all of the solid dissolved. Near the dissolution temperature, the temperature was increased at a rate of 0.2 K/20 min. Complete dissolution was determined using a laser monitoring system.

Source and Purity of Chemicals:

(1) 99+%, Chemical source not specified, no purification details were provided.

(2) 99+%, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.05 K.

x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[103]C. R. Daniels, A. K. Charlton, R. M. Wold, R. J. Moreno, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 633 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9826	0.01736

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 289 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9307	0.06932

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9173	0.08266

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9207	0.0793

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,3-Propanediol; $C_3H_8O_2$; [504-63-2]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9331	0.0669

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 1,2,3-Propanetriol (Glycerol); $C_3H_8O_3$; [60-29-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9282	0.07179

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

8.8. 4-Aminobenzoic acid solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-85-5]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8169	0.1831

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph. Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

8.9. 4-Aminobenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Propanone; C_3H_6O; [67-64-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9474	0.05265

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Acetophenone; C_8H_8O; [98-86-2]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9957	0.004335

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

8.10. 4-Aminobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9229	0.0771

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Propanoic acid; $C_3H_6O_2$; [79-09-4]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9510	0.0490

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Formamide; CH_3NO; [75-12-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9878	0.01223

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) *N,N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9991	0.000904

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) Butyl 2-hydroxypropanoate; $C_7H_{14}O_3$; [128-22-7]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9015	0.0985

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) Purity not given, Purac Inc., no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Aminobenzoic acid; $C_7H_7NO_2$; [150-13-0] (2) γ-Butyrolactone; $C_4H_6O_2$; [96-48-0]	[51]H.-M. Lin and R. A. Nash, J. Pharm. Sci. **82**, 1018 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8335	0.1665

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, and high-performance liquid chromatograph.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed with several turns of electrical tape, warmed to about 323 K, and then shaken in a constant-temperature bath for at least 24 h at 298 K. After equilibrium was reached, the sample was filtered through a 0.45 or 1.0 μm filter, and an aliquot was diluted appropriately for chromatographic analysis. Concentrations were determined by a high-performance liquid chromatographic method.

Source and Purity of Chemicals:
(1) Purity not given, Eastman Kodak Chemical Company, Rochester, NY, USA, no information provided concerning purification.
(2) Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

9. Solubility of 4-Amino-2-hydroxybenzoic Acid in Organic Solvents

9.1. Critical evaluation of experimental solubility data

There has been only a single publication that has reported solubility data for 4-amino-2-hydroxybenzoic acid. Takayama *et al.*[105] measured the solubility of 4-amino-2-hydroxybenzoic acid in 1,1′-oxybisethane as part of an experimental study aimed at studying the interactions between *N*-methyl-2-pyrrolidone and 4-aminobenzoic acids. Solubilities were measured as a function of *N*-methyl-2-pyrrolidone with 1,1′-oxybisethane serving as the solvent in the complexation study. 4-Amino-2-hydroxybenzoic acid and *N*-methyl-2-pyrrolidone were found to form a slightly soluble 1:1 association complex having a calculated stability constant of $K = 24.44\ \mathrm{dm}^3\ \mathrm{mol}^{-1}$. It is not possible to perform a critical evaluation of the experimental data as measurements were made at only a single temperature, and there is no independent experimental 4-amino-2-hydroxybenzoic acid solubility data in 1,1′-oxybisethane.

The experimental solubility data for 4-amino-2-hydroxybenzoic acid in 1,1′-oxybisethane is given in Sec. 9.2.

9.2. 4-Amino-2-hydroxybenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 4-Amino-2-hydroxybenzoic acid; $C_7H_7NO_3$; [65-49-6] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[105]P. K. Takayama, N. Nambu, and T. Nagai, Chem. Pharm. Bull. **25**, 879 (1977).
Variables: T/K = 283	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The solubility was given graphically as a plot of molar concentration of the solute versus the concentration of ligand added. From the graph, the compiler estimated a molar solubility of $c_1 = 0.076\ \mathrm{mol\,dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were sealed in vials and incubated for 48 h at 283 K. A 1 ml sample of the supernatant was withdrawn and the solvent evaporated at 323 K. The residue was dissolved in water or ethanol, and the concentration of the solute determined from spectroscopic absorbance measurements.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, was recrystallized from water before use.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: No information was given.

c_1: ±5% (relative error, estimated by compiler).

10. Solubility of 5-Amino-2-hydroxybenzoic Acid in Organic Solvents

10.1. Critical evaluation of experimental solubility data

There has been only a single publication that has reported solubility data for 5-amino-2-hydroxybenzoic acid. Patel *et al.*[107] measured the solubility of 5-amino-2-hydroxybenzoic acid in tetrahydrofuran, tetrachloromethane, methanol, and ethanol at 11 temperatures between 293 and 313 K. The internal consistency of the dataset was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 15, along with the root-mean-square deviation (RMSD) defined by

$$\mathrm{RMSD} = \left[\sum_{i=1}^{N} \frac{(x_1^{\,\mathrm{exp}} - x_1^{\,\mathrm{calc}})^2}{N-1}\right]^{1/2}, \tag{35}$$

and the MRD given by Eq. (24). In Eq. (35), N is the number of experimental solubility measurements in an individual solute-solvent data set. Examination of the entries in the last column of Table 15 reveals that the largest average relative deviation between the back-calculated values based on Eq. (8) and experimental data is less than 4%. Results of the mathematical representation analyses indicate that the experimental data for all four 5-amino-2-hydroxybenzoic acid – organic solvent systems are internally consistent.

The experimental solubility data for 5-amino-2-hydroxybenzoic acid in the different organic solvents are in Secs. 10.2–10.4.

10.2. 5-Amino-2-hydroxybenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 5-Amino-2-hydroxybenzoic acid; $C_7H_7NO_3$; [89-57-6] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[107]A. Patel, A. Vaghasiya, R. Gajera, and S. Baluja, J. Chem. Eng. Data **55**, 1453 (2010).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

TABLE 15. Parameters of the Modified Apelblat equation for describing the solubility of 5-amino-2-hydroxybenzoic acid in various organic solvents

Solvent	A	B	C	10^6 RMSD	MRD (%)
Tetrahydrofuran[a]	−0.9140	0.0024	−0.1237	17.9244	−3.86
Tetrachloromethane[a]	−9.3301	0.0118	0	0.2812	−0.14
Methanol[a]	−18.053	0.0399	0	0.1036	2.80
Ethanol[a]	−15.354	0.0313	0	0.0613	1.90

[a]Values of the coefficients, root-mean-square deviation, and mean relative deviation were taken from Patel *et al.*[107]

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.1845	0.8155
295.15	0.1803	0.8197
297.15	0.1764	0.8236
299.15	0.1724	0.8276
301.15	0.1683	0.8317
303.15	0.1643	0.8357
305.15	0.1603	0.8397
307.15	0.1562	0.8438
309.15	0.1521	0.8479
311.15	0.1480	0.8520
313.15	0.1440	0.8560

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath, stirrer, and analytical balance. Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in an equilibrium cell and allowed to equilibrate in a constant-temperature water bath with continuous stirring for at least 3 h. The stirring was then stopped and the solution was allowed to equilibrate an additional 2 h to allow suspended solid to settle to the bottom of the container. An aliquot of the saturated solution was removed, filtered, and transferred to a tared vial. The vial was tightly closed and quickly weighed to determine the amount of sample transferred. The vial was then opened and the solvent allowed to evaporate at ambient room temperature. After the solvent had evaporated, the vial was dried and reweighed. The solubility was calculated from the mass of the solid residue and mass of sample transferred.

Source and Purity of Chemicals:
(1) 99.5%, Hiran Orgochem Ltd., Ankleshwar, India, was recrystallized before use.
(2) Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±<1.0% (relative error).

10.3. 5-Amino-2-hydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 5-Amino-2-hydroxybenzoic acid; $C_7H_7NO_3$; [89-57-6] (2) Tetrachloromethane; CCl_4; [56-23-5]	[107] A. Patel, A. Vaghasiya, R. Gajera, and S. Baluja, J. Chem. Eng. Data **55**, 1453 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9971	0.002902
295.15	0.9970	0.003027
297.15	0.9969	0.003098
299.15	0.9969	0.003116
301.15	0.9968	0.003159
303.15	0.9968	0.003187
305.15	0.9967	0.003313
307.15	0.9966	0.003446
309.15	0.9964	0.003619
311.15	0.9963	0.003705
313.15	0.9962	0.003827

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath, stirrer, and analytical balance. Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in an equilibrium cell and allowed to equilibrate in a constant-temperature water bath with continuous stirring for at least 3 h. The stirring was then stopped and the solution was allowed to equilibrate an additional 2 h to allow suspended solid to settle to the bottom of the container. An aliquot of the saturated solution was removed, filtered, and transferred to a tared vial. The vial was tightly closed and quickly weighed to determine the amount of sample transferred. The vial was then opened and the solvent allowed to evaporate at ambient room temperature. After the solvent had evaporated, the vial was dried and reweighed. The solubility was calculated from the mass of the solid residue and mass of sample transferred.

Source and Purity of Chemicals:
(1) 99.5%, Hiran Orgochem Ltd., Ankleshwar, India, was recrystallized before use.
(2) Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±<3.0% (relative error).

10.4. 5-Amino-2-hydroxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 5-Amino-2-hydroxybenzoic acid; $C_7H_7NO_3$; [89-57-6] (2) Methanol; CH_4O; [67-56-1]	[107] A. Patel, A. Vaghasiya, R. Gajera, and S. Baluja, J. Chem. Eng. Data **55**, 1453 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9986	0.001408
295.15	0.9984	0.001551
297.15	0.9983	0.001705
299.15	0.9981	0.001876
301.15	0.9980	0.002018
303.15	0.9978	0.002154
305.15	0.9976	0.002401
307.15	0.9974	0.002642
309.15	0.9922	0.002837
311.15	0.9970	0.003021
313.15	0.9968	0.003162

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath, stirrer, and analytical balance. Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in an equilibrium cell and allowed to equilibrate in a constant-temperature water bath with continuous stirring for at least 3 h. The stirring was then stopped and the solution was allowed to equilibrate an additional 2 h to allow suspended solid to settle to the bottom of the container. An aliquot of the saturated solution was removed, filtered, and transferred to a tared vial. The vial was tightly closed and quickly weighed to determine the amount of sample transferred. The vial was then opened and the solvent allowed to evaporate at ambient room temperature. After the solvent had evaporated, the vial was dried and reweighed. The solubility was calculated from the mass of the solid residue and mass of sample transferred.

Source and Purity of Chemicals:
(1) 99.5%, Hiran Orgochem Ltd., Ankleshwar, India, was recrystallized before use.
(2) Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±<3.0% (relative error).

Components:	**Original Measurements:**
(1) 5-Amino-2-hydroxybenzoic acid; $C_7H_7NO_3$; [89-57-6] (2) Ethanol; C_2H_6O; [64-17-5]	[107]A. Patel, A. Vaghasiya, R. Gajera, and S. Baluja, J. Chem. Eng. Data **55**, 1453 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9982	0.001765
295.15	0.9981	0.001931
297.15	0.9979	0.002117
299.15	0.9977	0.002254
301.15	0.9977	0.002334
303.15	0.9975	0.002491
305.15	0.9973	0.002738
307.15	0.9971	0.002946
309.15	0.9969	0.003087
311.15	0.9968	0.003227
313.15	0.9965	0.003454

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath, stirrer, and analytical balance. Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in an equilibrium cell and allowed to equilibrate in a constant-temperature water bath with continuous stirring for at least 3 h. The stirring was then stopped and the solution was allowed to equilibrate an additional 2 h to allow suspended solid to settle to the bottom of the container. An aliquot of the saturated solution was removed, filtered, and transferred to a tared vial. The vial was tightly closed and quickly weighed to determine the amount of sample transferred. The vial was then opened and the solvent allowed to evaporate at ambient room temperature. After the solvent had evaporated, the vial was dried and reweighed. The solubility was calculated from the mass of the solid residue and mass of sample transferred.

Source and Purity of Chemicals:
(1) 99.5%, Hiran Orgochem Ltd., Ankleshwar, India, was recrystallized before use.
(2) Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±<4.0% (relative error).

11. Solubility of 1,2-Benzenedicarboxylic Acid in Organic Solvents

11.1. Critical evaluation of experimental solubility data

Several research groups[50,60,76,79,108–111] have investigated the solubility behavior of 1,2-benzenedicarboxylic acid as a function of temperature. Ren *et al.*[108] employed a dynamic method with laser monitoring to study the solubility of 1,2-benzenedicarboxylic acid in butyl ethanoate and methanol. Che *et al.*[109] determined the solubility of 1,2-benzenedicarboxylic acid in tetrahydrofuran, 1,2-diethoxyethane, cyclohexanone, and acetophenone at several temperatures.

The internal consistency of the six datasets of measured 1,2-benzenedicarboxylic acid solubilities was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 16, along with the MRD calculated according to Eq. (24). Examination of the numerical entries in the last column of Table 16 reveals that the largest mean relative deviation between the back-calculated values based on Eq. (8) and experimental data is only 0.8%, which is less than the experimental uncertainties in the measured values. Results of the mathematical representation analyses indicate that the

TABLE 16. Parameters of the Modified Apelblat equation for describing the solubility of 1,2-benzenedicarboxylic acid in various organic solvents

Solvent	*A*	*B*	*C*	MRD (%)
Butyl ethanoate[a]	−146.09	4646.2	21.836	0.82
Methanol[a]	15.381	−2208.7	−1.9198	0.03
1,2-Diethoxyethane[b]	−59.994	1482.7	8.9357	0.44
Tetrahydrofuran[b]	−78.560	2796.4	11.682	0.31
Cyclohexanone[b]	−78.708	1933.1	11.984	0.70
Acetophenone[b]	−78.865	1321.7	12.131	0.29

[a] Values of the coefficients and the mean relative deviations were taken from Ren *et al.*[108]

[b] Values of the coefficients and the mean relative deviations were taken from Che *et al.*[109]

experimental data for all six 1,2-benzenedicarboxylic acid – organic solvent systems are internally consistent.

Zhao *et al.*[60] measured the solubility of 1,2-benzenedicarboxylic acid in isobutyl ethanoate at 12 temperatures between 301 and 349 K. The experimental data were correlated with the UNIQUAC model. Interaction coefficients calculated from the experimental solid-liquid equilibrium data provided a reasonably accurate mathematical description of the measured values. The mean absolute relative deviation between calculated and observed values was less than 6.4%.

The experimental solubility data for 1,2-benzenedicarboxylic acid in the different organic solvents are in Secs. 11.2–11.9.

11.2. 1,2-Benzenedicarboxylic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Benzene; C_6H_6; [71-43-2]	[50] P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000447

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, no information provided concerning purification.

(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:

Temperature: No information given.

x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Methylbenzene; C_7H_8; [108-88-8]	[50] P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000465

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, no information provided concerning purification.

(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:

Temperature: No information given.

x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]	[50] P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000465

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

11.3. 1,2-Benzenedicarboxylic acid solubility data in esters

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[108]B.-Z. Ren, C.-H. Hou, H.-G. Chong, W.-R. Li, and H.-J. Song, J. Chem. Eng. Data **51**, 2022 (2006).
Variables:	**Prepared by:**
Temperature; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
304.89	0.9972	0.002753
310.12	0.9970	0.002958
315.87	0.9967	0.003294
320.35	0.9964	0.003640
325.33	0.9959	0.004080
330.25	0.9954	0.004587
334.75	0.9949	0.005060
338.99	0.9944	0.005583
341.55	0.9939	0.006117
345.83	0.9933	0.006724
352.01	0.9922	0.007751
356.07	0.9915	0.008515
359.75	0.9906	0.009362

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermoelectric circulating water temperature controller, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.8%, CP grade, Shanghai Chemical Reagent Research Institute, China, no purification details were provided.
(2) 99.0%, Analytical Reagent grade, Tianjing Huadong Chemical Reagent Factory, distilled prior to use.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.001.

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Isobutyl ethanoate; $C_6H_{12}O_2$; [110-19-0]	[60]S. Zhao, X. Chen, Q. Dai, and L. Wang, J. Chem. Eng. Data **56**, 2399 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
300.68	0.9989	0.0011
302.37	0.9988	0.0012
304.42	0.9988	0.0012
309.58	0.9984	0.0016
312.72	0.9978	0.0022
317.36	0.9974	0.0026
326.85	0.9968	0.0032
331.86	0.9963	0.0037
335.27	0.9950	0.0050
340.04	0.9938	0.0062
342.69	0.9923	0.0077
348.70	0.9908	0.0092

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermoelectric circulating water temperature controller, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate 1–2 K/h (0.5–1.0 K/h or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.
(2) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0002.

11.4. 1,2-Benzenedicarboxylic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.25	0.9303	0.06973
303.15	0.9246	0.07543
313.45	0.9174	0.08263
323.15	0.9101	0.08991
329.05	0.9051	0.09493

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99.8%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99%, Kermel Chemical Reagents Development Centre, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) 1,2-Diethoxyethane; $C_6H_{14}O_2$; [629-14-1]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9846	0.01544
303.25	0.9823	0.01767
313.20	0.9800	0.02003
323.05	0.9772	0.02283
333.15	0.9739	0.02613
343.05	0.9698	0.03017

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99.8%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

11.5. 1,2-Benzenedicarboxylic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9998	0.000184

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Tetrachloromethane; CCl_4; [56-23-5]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: $T/K = 301.2$	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000244

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: $T/K = 301.2$	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000577

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

11.6. 1,2-Benzenedicarboxylic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Methanol; CH_4O; [67-56-1]	[108]B.-Z. Ren, C.-H. Hou, H.-G. Chong, W.-R. Li, and H.-J. Song, J. Chem. Eng. Data **51**, 2022 (2006).
Variables: Temperature; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
302.67	0.9441	0.05591
305.75	0.9410	0.05902
308.63	0.9379	0.06209
311.55	0.9349	0.06513
314.35	0.9318	0.06817
317.03	0.9288	0.07121
319.71	0.9257	0.07427
322.29	0.9227	0.07730
324.85	0.9197	0.08034
327.35	0.9166	0.08342
329.83	0.9135	0.08650
332.25	0.9105	0.08953

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermoelectric circulating water temperature controller, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.8%, CP grade, Shanghai Chemical Reagent Research Institute, China, no purification details were provided.
(2) 99.5%, Analytical Reagent grade, Tianjing Huadong Chemical Reagent Factory, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.001.

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Methanol; CH_4O; [67-56-1]	[110]M. K. Chantooni, Jr. and I. M. Kolthoff, J. Phys. Chem. **79**, 1176 (1975).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.15 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Matheson Coleman and Bell, USA, was recrystallized from acetonitrile.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Methanol; CH_4O; [67-56-1]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9487	0.05125

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Ethanol; C_2H_6O; [64-17-5]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9573	0.04265

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) 1-Propanol; C_3H_8O; [71-23-8]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9727	0.02732

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9777	0.02231

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.354 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Matheson Coleman and Bell, USA, was recrystallized from acetonitrile.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[111]B. K. Dolui, S. K. Bhattacharya, and K. K. Kundu, J. Solution Chem. **37**, 987 (2008).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9533	0.04669

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility was reported in the paper as 0.789 mol/kg of solvent. Mole fraction value calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Mechanical shaker and a thermostated temperature control system.
Excess solute and solvent were placed in a well-stoppered bottle and shaken in a mechanical shaker at low speed for 12 h at ambient room temperature. The bottle was then thermostated at 298 K for several days for the solution to reach equilibrium. Aliquots of the solution were withdrawn every two days by a specially constructed pipette fitted with G3-Gooch disk, and then weighed. The concentration in the saturated solution was determined by titrating with standardized potassium hydroxide solution using phenolphthalein as the endpoint indicator. The equilibration and analysis continued until successive readings agreed to within ±1%.

Source and Purity of Chemicals:
(1) G.R. grade, Merck Chemical Company, Germany, was used as received.
(2) L.R. grade, BDH Chemicals, was purified by methods detailed in an earlier publication [B. K. Dolui, S. K. Bhattacharya, and S. S. Kundu, Indian J. Chem. Sect. A **45A**, 2607 (2006)].

Estimated Error:
Temperature: ± 0.01 K.
x_1: ±1% (relative error).

11.7. 1,2-Benzenedicarboxylic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Propanone; C_3H_6O; [67-64-1]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9710	0.02896

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9824	0.01763
303.15	0.9788	0.02117
313.15	0.9743	0.02568
323.15	0.9690	0.03096
333.15	0.9630	0.03697
343.40	0.9541	0.04591

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system. Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99.8%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Acetophenone; C_8H_8O; [98-86-2]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.35	0.9944	0.005601
313.35	0.9928	0.007236
323.35	0.9907	0.009333
332.95	0.9881	0.01186
343.55	0.9848	0.01525

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system. Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99.8%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

11.8. 1,2-Benzenedicarboxylic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[79]Q. Wang, L. Hou, Y. Cheng, and X. Li, J. Chem. Eng. Data **52**, 936 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.3	0.9894	0.0106
308.4	0.9850	0.0150
318.3	0.9778	0.0222
328.2	0.9692	0.0308
338.0	0.9583	0.0417
348.3	0.9443	0.0557
358.6	0.9278	0.0722
367.9	0.9095	0.0905

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.
[c] Solubility data were given in units of grams per 100 g of solvent. Mole fraction solubilities were calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and analytical balance.
Solubilities were determined by a static method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h. An aliquot of the clear solution was removed by syringe and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was evaporated in *in vacuo* at 323 K for more than 3 h. Once the solvent had evaporated, the vial with solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 98.5%, Shanghai Fine Chemical Reagent Company, China, no purification details provided.
(2) Analytical Reagent grade, Hangzhou Chemical Reagent Company, China, no purification details provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[110]M. K. Chantooni, Jr. and I. M. Kolthoff, J. Phys. Chem. **79**, 1176 (1975).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.0245 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Matheson Coleman and Bell, USA, was recrystallized from acetonitrile.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[110]M. K. Chantooni, Jr. and I. M. Kolthoff, J. Phys. Chem. **79**, 1176 (1975).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 3.77 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Matheson Coleman and Bell, USA, was recrystallized from acetonitrile.
(2) Purity not given, Chemical Source not given, was shaken with activated alumina and then distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000898

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

11.9. 1,2-Benzenedicarboxylic acid solubility data in binary organic solvent mixtures

Components:	**Original Measurements:**
(1) 1,2-Benzenedicarboxylic acid; $C_8H_6O_4$; [88-99-3] (2) Methanol; CH_4O; [67-56-1] (3) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[108]B.-Z. Ren, C.-H. Hou, H.-G. Chong, W.-R. Li, and H.-J. Song, J. Chem. Eng. Data **51**, 2022 (2006).
Variables:	**Prepared by:**
Temperature; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	$m_2^{(s)}$[a]	x_1[b]
304.89	0.0000	0.002753
310.12	0.0000	0.002958
315.87	0.0000	0.003294
320.35	0.0000	0.003640
325.33	0.0000	0.004080
330.25	0.0000	0.004587
334.75	0.0000	0.005060
338.99	0.0000	0.005583
341.55	0.0000	0.006117
345.83	0.0000	0.006724
352.01	0.0000	0.007751
356.07	0.0000	0.008515
359.75	0.0000	0.009362
303.10	0.1997	0.01863
305.82	0.1997	0.01953
309.65	0.1997	0.02082
313.56	0.1997	0.02182
316.52	0.1997	0.02276
320.44	0.1997	0.02377
324.07	0.1997	0.02478
327.66	0.1997	0.02586
332.67	0.1997	0.02704
334.30	0.1997	0.02792
304.57	0.3992	0.03555
307.20	0.3992	0.03711
310.62	0.3992	0.03879
314.04	0.3992	0.04053
317.66	0.3992	0.04230
320.77	0.3992	0.04409
324.25	0.3992	0.04592
327.82	0.3992	0.04783
330.86	0.3992	0.04981
334.26	0.3992	0.05187
300.46	0.6001	0.04255
303.37	0.6001	0.04471
306.50	0.6001	0.04687
309.74	0.6001	0.04906
312.88	0.6001	0.05125
315.77	0.6001	0.05344
318.86	0.6001	0.05573
321.70	0.6001	0.05792
324.82	0.6001	0.06020
327.74	0.6001	0.06248
330.77	0.6001	0.06480
333.94	0.6001	0.06717
303.62	0.8000	0.05167
306.24	0.8000	0.05412
309.46	0.8000	0.05662
312.13	0.8000	0.05910
315.22	0.8000	0.06168
317.91	0.8000	0.06429
320.96	0.8000	0.06696
324.22	0.8000	0.06975
326.24	0.8000	0.07268
328.99	0.8000	0.07576
332.06	0.8000	0.07901
335.20	0.8000	0.08247
302.67	1.0000	0.05591
305.75	1.0000	0.05902
308.63	1.0000	0.06209
311.55	1.0000	0.06513
314.35	1.0000	0.06817
317.03	1.0000	0.07121
319.71	1.0000	0.07427
322.29	1.0000	0.07730
324.85	1.0000	0.08034
327.35	1.0000	0.08342
329.83	1.0000	0.08650
332.25	1.0000	0.08953

[a] $m_2^{(s)}$: mass fraction of component 2 in the initial binary solvent mixture.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermoelectric circulating water temperature controller, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.8%, CP grade, Shanghai Chemical Reagent Research Institute, China, no purification details were provided.
(2) 99.5%, Analytical Reagent grade, Tianjing Huadong Chemical Reagent Factory, China, no purification details were provided.
(3) 99.0%, Analytical Reagent grade, Tianjing Huadong Chemical Reagent Factory, was distilled prior to use.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
$m_2^{(s)}$: 0.0001
x_1: ±0.001.

12. Solubility of 1,3-Benzenedicarboxylic Acid in Organic Solvents

12.1. Critical evaluation of experimental solubility data

Several research groups[60,63,82,84,91,109,112–117] have investigated the solubility behavior of 1,3-benzenedicarboxylic acid as a function of temperature. Che *et al.*[109] determined the solubility of 1,3-benzenedicarboxylic acid in tetrahydrofuran, 1,2-diethoxyethane, cyclohexanone, and acetophenone at several temperatures. The internal consistency of the four sets of measured 1,3-benzenedicarboxylic acid solubilities were assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 17, along with the MRD calculated according to Eq. (24). Examination of the entries in the last column of Table 17 reveals that the largest mean relative deviation between the back-calculated values based on Eq. (8) and experimental data is only 1.2%,which is less than the experimental uncertainties in the measured values. Results of

TABLE 17. Parameters of the Modified Apelblat equation for describing the solubility of 1,3-benzenedicarboxylic acid in various organic solvents

Solvent	A	B	C	MRD (%)
1,2-Diethoxyethane[a]	−139.95	5175.9	20.483	0.17
Tetrahydrofuran[a]	−79.312	2713.1	11.583	0.20
Cyclohexanone[a]	−58.711	679.31	8.8686	1.18
Acetophenone[a]	−272.87	10667	40.328	0.59

[a]Values of the coefficients and the mean relative deviations were taken from Che *et al.*[109]

the mathematical representation analyses indicate that the experimental data for all four 1,3-benzenedicarboxylic acid – organic solvent systems are internally consistent.

Long *et al.*[112] used a gravimetric method to examine the solubility behavior of 1,3-benzenedicarboxylic acid in seven monobasic alcohols (methanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 1-pentanol, and 1-hexanol) in the temperature range of about 278–352 K. Long and Yang[116] had previously measured the solubility of 1,3-benzenedicarboxylic acid in ethanol, propanone, and ethyl ethanoate. For the alcohol solvents, solubilities were found to decrease with increasing number of carbon atoms, except for 1-pentanol where the solubility was comparable to that observed in 1-butanol and higher than the measured solubility in 2-butanol. Methanol exhibited the highest ability to dissolve the dicarboxylic acid solute, whereas 1-hexanol showed the lowest solubility. The internal consistency of the ten datasets of measured 1,3-benzenedicarboxylic acid solubilities mentioned above, along with the measured values of Feng *et al.*[117] for 1,3-benzenedicarboxylic acid dissolved in ethanoic acid, were assessed by curve-fitting the measured mole fraction solubility data to Eq. (9). The values of the equation coefficients (λ and h) are given in Table 18, along with the MRD.

TABLE 18. Parameters of the Buchowski λh equation for describing the solubility of 1,3-benzenedicarboxylic acid in several organic solvents

Solvent	T/K	λ	$10^{-4}\,h$	MRD (%)
Methanol[a]	278–337	0.1016	1.865	2.62
Ethanol[b]	278–350	0.1696	1.223	1.57
1-Propanol[a]	278–358	0.3630	0.7471	4.05
2-Propanol[a]	278–353	0.4151	0.6431	2.01
1-Butanol[a]	278–358	0.2366	1.049	4.33
2-Butanol[a]	283–352	0.2356	1.124	3.80
1-Pentanol[a]	303–348	0.2362	1.000	3.03
1-Hexanol[a]	278–353	0.3793	0.7523	3.52
Propanone[b]	278–328	1.2853	0.2840	2.62
Ethyl ethanoate[b]	278–338	0.0658	4.1360	9.87
Ethanoic acid[c]	313–363	0.0434	6.7978	3.72

[a]Values of the coefficients and mean relative deviations were taken from Long *et al.*[112]

[b]Values of the coefficients and mean relative deviations were taken from Long and Yang.[116]

[c]Values of the coefficients and mean relative deviation were taken from Feng *et al.*[113]

Zhao *et al.*[60] measured the solubility of 1,3-benzenedicarboxylic acid in isobutyl ethanoate at ten temperatures between 308 and 353 K. The experimental data were correlated with both the UNIQUAC and Wilson models. Interaction coefficients calculated from the experimental solid-liquid equilibrium data provided a reasonably accurate mathematical description of the measured values. The mean absolute relative deviation between calculated and observed values was 11.56% (Wilson model) and 10.90% (UNIQUAC model).

Li *et al.*[84] determined the solubility of 1,3-benzenedicarboxylic acid in *N*-methyl-2-pyrrolidone from 296 to 346 K using a synthetic method with laser monitoring to determine when the last amount of solid solute dissolved. The authors employed a polynomial expression in temperature

$$x_1 = -6.9703 + 0.06877\,T - 2.29731 \times 10^{-4}\,T + 2.63346 \times 10^{-7} T^2 \tag{36}$$

to represent the measured mole fraction solubility data. The root-mean-square deviation between the observed x_1 data and calculated values from Eq. (36) was on the order of 0.0014 mole fraction.

Feng *et al.*[113] studied the water-to-propyl ethanoate partitioning behavior of 1,3-benzenedicarboxylic acid as well as the solute's solubility in propyl ethanoate from 303 to 363 K. The authors described the logarithm of the observed mole fraction solubilities with a simple linear relationship

$$\log_{10} x_1 = -5.2411 + 0.00705 T. \tag{37}$$

The mean absolute deviation between the observed mole fraction solubilities and back-calculated values based on Eq. (37) was less than 2.6%.

The experimental solubility data for 1,3-benzenedicarboxylic acid in the different organic solvents are in Secs. 12.2–12.6.

12.2. 1,3-Benzenedicarboxylic acid solubility data in esters

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[116]B. Long and Z. Yang, Fluid Phase Equilib. **266**, 38 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	$100s_1$[a]
278.05	0.2754
282.95	0.3939
287.85	0.5311
293.05	0.6039
303.05	0.8864
307.75	1.0034
312.85	1.0819
323.65	1.3660
333.15	1.6203
338.15	1.7177

[a] s_1: solubility of the solute in units of moles per kilogram. The authors description of how the solubilities are reported is contradictory. In the manuscript text, the authors state molarity, and moles per kilogram of solution. Compiler has assumed that the units are moles per kilogram, which would be consistent with the column heading of the table in the published paper.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed equilibrium cell, constant-temperature circulating water bath, analytical balance, oven, and magnetic stirrer.

Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for at least 5 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet, and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:

(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.

(2) 99.5%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:

Temperature: ±0.1 K.

s_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[113]L. Feng, L. Wang, G. Peng, X. Guo, and X. Li, J. Chem. Eng. Data **55**, 500 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.2	0.9992	0.000791
313.2	0.9991	0.000934
323.2	0.9989	0.001082
333.2	0.9987	0.001321
343.2	0.9986	0.001379
353.2	0.9982	0.001797
363.2	0.9979	0.002145

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Thermoelectric temperature controlling system and a high-performance liquid chromatograph.

Experimental solubilities were determined by a static method. A sealed bottle containing excess solute and solvent was allowed to equilibrate at constant temperature for at least 24 h. A 3 ml aliquot of the saturated solution was removed with a preheated syringe, and injected into a test tube which contained 3 ml of dimethyl sulfoxide. The concentration of the solute was determined by high-performance liquid chromatographic method.

Source and Purity of Chemicals:

(1) 98%, Tokyo Kasei Kogyo Company, Ltd., Japan, used as received.

(2) 99%, Hangzhou Chemical Reagent Company, China, used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) Isobutyl ethanoate; $C_6H_{12}O_2$; [110-19-0]	[60]S. Zhao, X. Chen, Q. Dai, and L. Wang, J. Chem. Eng. Data **56**, 2399 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
308.15	0.9996	0.000352
313.15	0.9996	0.000388
318.15	0.9996	0.000438
323.15	0.9995	0.000507
328.15	0.9993	0.000691
333.15	0.9991	0.000917
338.15	0.9987	0.001300
343.15	0.9983	0.001663
348.15	0.9980	0.002009
353.15	0.9978	0.002209

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated temperature controller, electromagnetic stirrer, analytical balance, an ultraviolet-visible spectrophotometer.
Experimental solubilities were determined by a static method. A sealed flask containing excess solute and solvent was allowed to equilibrate at constant temperature with continuous stirring for 2 h. The stirring was stopped and the excess solid was permitted to settle to the bottom of the flask. Aliquots of the saturated solution were removed, diluted quantitatively with isobutyl ethanoate, and the absorbance recorded at 280 nm. The solubility was calculated based on the Beer-Lambert law using measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.
(2) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.00005.

12.3. 1,3-Benzenedicarboxylic acid solubilities in ethers

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.984	0.016

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.7% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.35	0.9859	0.01414
303.15	0.9846	0.01541
313.45	0.9831	0.01693
322.85	0.9815	0.01849
328.75	0.9804	0.01956

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99%, Kermel Chemical Reagents Development Centre, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

Components:	Original Measurements:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.994	0.006

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3.6% (relative error).

Components:	Original Measurements:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1,2-Diethoxyethane; $C_6H_{14}O_2$; [629-14-1]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.30	0.9973	0.002651
303.15	0.9971	0.002929
313.15	0.9967	0.003297
322.75	0.9962	0.003759
332.65	0.9957	0.004331
342.45	0.9950	0.005017

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

12.4. 1,3-Benzenedicarboxylic acid solubility data in alcohols

Components:	Original Measurements:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) Methanol; CH_4O; [67-56-1]	[114]G. N. Friedlin and V. N. Davydov, Zh. Prikl. Khim. **35**, 2530 (1962).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

The authors report a solubility of 1.753 g of solute per 100 ml of solvent at 293 K, and a solubility of 3.990 g of solute per 100 ml of solvent at 338 K.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details were not provided.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
Solubility: ± 1% (relative error).

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
[115]G. N. Freidlin and V. N. Davydov, Dopov. Akad. Nauk Ukr. RSR 622 (1962).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9957	0.00426
313	0.9937	0.00633
323	0.9924	0.00758
330	0.9917	0.00834
337	0.9895	0.01051

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were expressed as grams of solute per 100 g of solvent. Mole fraction values calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details were not provided.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
x_1: ±2% (relative error).

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
[112]B. Long, Y. Wang, R. Zhang, and J. Xu, J. Chem. Eng. Data **54**, 1764 (2009).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.9975	0.002530
283.25	0.9972	0.002755
288.05	0.9969	0.003142
293.25	0.9965	0.003455
298.75	0.9962	0.003787
302.65	0.9959	0.004110
307.95	0.9954	0.004555
313.45	0.9949	0.005118
318.45	0.9942	0.005784
323.25	0.9934	0.006589
328.25	0.9929	0.007144
333.15	0.9921	0.007913
337.25	0.9912	0.008823

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium cell, constant-temperature circulating water bath, analytical balance, oven, and magnetic stirrer.
Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for 2 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.
(2) 99+%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error).

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
[116]B. Long and Z. Yang, Fluid Phase Equilib. **266**, 38 (2008).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	$100s_1$[a]
278.54	6.2361
283.33	6.9042
288.33	7.8402
293.05	8.9950
297.45	9.8858
302.66	10.6423
308.55	12.7611
313.15	13.9168
318.45	15.7286
323.45	16.8814
328.15	18.4253
333.05	20.9806
338.15	22.9459
343.65	25.9315
349.35	29.3565

[a] s_1: solubility of the solute in units of moles per kilogram. The authors' description of how the solubilities are reported is contradictory. In the manuscript text, the authors state molarity, and moles per kilogram of solution. Compiler has assumed that the units are moles per kilogram, which would be consistent with the column heading of the table in the published paper.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.
Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for at least 5 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.
(2) 99.5%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.1 K.
s_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1-Propanol; C_3H_8O; [71-23-8]	[112]B. Long, Y. Wang, R. Zhang, and J. Xu, J. Chem. Eng. Data **54**, 1764 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.9983	0.001685
280.84	0.9981	0.001901
283.34	0.9978	0.002198
288.17	0.9975	0.002493
293.15	0.9973	0.002677
298.35	0.9968	0.003205
304.05	0.9962	0.003769
308.25	0.9958	0.004248
313.15	0.9953	0.004731
317.55	0.9947	0.005281
320.17	0.9944	0.005636
323.50	0.9933	0.006461
328.20	0.9929	0.007128
333.15	0.9914	0.008576
338.15	0.9903	0.009711
342.65	0.9895	0.01047
349.05	0.9878	0.01215
349.37	0.9875	0.01245
353.55	0.9852	0.01480
358.75	0.9826	0.01744

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.
Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for 2 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.
(2) 99+%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1-Propanol; C_3H_8O; [71-23-8]	[115]G. N. Freidlin and V. N. Davydov, Dopov. Akad. Nauk Ukr. RSR 622 (1962).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9941	0.00590
323	0.9901	0.00994
343	0.9877	0.01234
370	0.9751	0.02492

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were expressed as grams of solute per 100 g of solvent. Mole fraction values calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details were not provided.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
x_1: ±10% for 293 K value, less than 2% at the other temperatures (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 2-Propanol; C_3H_8O; [67-63-0]	[112]B. Long, Y. Wang, R. Zhang, and J. Xu, J. Chem. Eng. Data **54**, 1764 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.55	0.9978	0.002185
279.87	0.9977	0.002260
283.25	0.9974	0.002550
288.15	0.9991	0.002910
293.15	0.9967	0.003253
298.15	0.9960	0.003961
303.05	0.9954	0.004594
308.25	0.9947	0.005346
313.15	0.9939	0.006074
318.25	0.9932	0.006754
319.56	0.9930	0.007035
323.95	0.9919	0.008105
328.15	0.9909	0.009110
333.15	0.9898	0.01020
338.35	0.9889	0.01105
343.25	0.9866	0.01343
348.15	0.9852	0.01477
349.85	0.9849	0.01513
353.15	0.9828	0.01715

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.
Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for 2 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.
(2) 99+%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[112]B. Long, Y. Wang, R. Zhang, and J. Xu, J. Chem. Eng. Data **54**, 1764 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.06	0.9981	0.001872
283.11	0.9978	0.002157
288.27	0.9977	0.002339
293.30	0.9974	0.002649
298.06	0.9969	0.003149
303.66	0.9963	0.003664
308.36	0.9961	0.003860
312.66	0.9953	0.004736
317.94	0.9948	0.005200
322.25	0.9943	0.005661
328.54	0.9939	0.006333
334.57	0.9923	0.007655
337.96	0.9918	0.008166
338.64	0.9911	0.008924
343.20	0.9905	0.009537
347.67	0.9889	0.01106
353.44	0.9870	0.01304
358.67	0.9856	0.01437

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.
Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for at least 5 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.
(2) 99+%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[91]J. Bradil, J. Malek, and V. Bazant, Chem. Prumysl **20**, 117 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
273.2	0.9977	0.00225
298.2	0.9942	0.00575
323.2	0.9921	0.00788
343.6	0.9877	0.01228
358.2	0.9823	0.01774
362.7	0.9785	0.02151

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data were reported in terms of grams of dissolved solute per 100 g of solution. Mole fraction solubilities calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent and were placed in a flask and equilibrated at constant temperature with stirring. After 90 min the stirring was discontinued, and the solution was allowed to stand for 30 min to allow the undissolved solid to settle to the bottom of the flask. An aliquot of the saturated solution was removed by pipette fitted with a filtering device. The mass of the aliquot was determined by weighing. The concentration of the dissolved solute was determined by titration using sodium hydroxide, with phenolphthalein being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Amoco Chemical Corporation, Chicago, IL, USA, recrystallized three times from a mixture of methylbenzene and tetrachloromethane.
(2) Purity not given, Spolana, Neratovice, Czechoslovakia, was distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[112]B. Long, Y. Wang, R. Zhang, and J. Xu, J. Chem. Eng. Data **54**, 1764 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.05	0.9985	0.001455
288.05	0.9983	0.001721
293.15	0.9979	0.002085
298.25	0.9977	0.002349
303.45	0.9974	0.002625
308.25	0.9969	0.003113
313.25	0.9965	0.003457
318.15	0.9961	0.003910
322.95	0.9959	0.004134
327.95	0.9950	0.005035
332.65	0.9944	0.005634
337.55	0.9932	0.006785
342.25	0.9925	0.007479
347.35	0.9913	0.008695
350.65	0.9904	0.009585
352.65	0.9898	0.01023

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.
Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for at least 5 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.
(2) 99+%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[112]B. Long, Y. Wang, R. Zhang, and J. Xu, J. Chem. Eng. Data **54**, 1764 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.05	0.9959	0.004081
308.05	0.9947	0.005323
313.15	0.9941	0.005935
318.15	0.9935	0.006513
323.05	0.9926	0.007402
328.15	0.9918	0.008232
334.95	0.9906	0.009400
340.35	0.9897	0.01028
344.25	0.9883	0.01173
348.85	0.9877	0.01232

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.

Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for at least 5 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:

(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.

(2) 99+%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[112]B. Long, Y. Wang, R. Zhang, and J. Xu, J. Chem. Eng. Data **54**, 1764 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.48	0.9976	0.002435
302.97	0.9968	0.003204
308.15	0.9964	0.003617
312.70	0.9958	0.004235
317.67	0.9952	0.004766
320.84	0.9946	0.005439
326.96	0.9941	0.005930
332.56	0.9926	0.007372
337.65	0.9914	0.008570
343.76	0.9906	0.009458
349.25	0.9896	0.01042
353.94	0.9884	0.01159

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.

Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for at least 5 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:

(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.

(2) 99+%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±2% (relative error).

12.5. 1,3-Benzenedicarboxylic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5] (2) Propanone; C_3H_6O; [67-64-1]	[116]B. Long and Z. Yang, Fluid Phase Equilib. **266**, 38 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	$100s_1$[a]
278.25	1.7634
283.05	1.9788
288.05	2.4777
292.95	2.7495
297.65	3.5875
303.05	4.2633
308.05	5.3245
313.05	6.6758
318.05	8.0520
323.05	9.9103
327.85	12.3663

[a] s_1: solubility of the solute in units of moles per kilogram. The authors' description of how the solubilities are reported is contradictory. In the manuscript text, the authors state molarity, and moles per kilogram of solution. Compiler has assumed that the units are moles per kilogram, which would be consistent with the column heading of the table in the published paper.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed equilibrium cell, constant temperature circulating water bath, analytical balance, oven, and magnetic stirrer.

Excess solute and solvent were placed in a jacketed equilibrium cell and allowed to equilibrate with stirring at constant temperature for at least 5 h. After sufficient equilibration, the stirrer was stopped and the solution was kept still for at least 1 h to allow suspended solid to settle to the bottom of the cell. An aliquot of the clear upper saturated solution was removed with a warm pipet and transferred to a weighed vial. The vial was weighed, uncovered, and placed in an oven. The solvent was allowed to evaporate in the oven at 323 K. The vial was covered with a piece of filter cloth to prevent dust contamination. After the solvent had evaporated, the vial was reweighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:

(1) 99.8%, Beijing Yanshan Petrochemical Company, China, no purification details provided.

(2) 99.5%, Beijing Chemical Reagent Company, China, used as received.

Estimated Error:
Temperature: ±0.1 K.
s_1: ±2% (relative error).

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]

Original Measurements:
[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.35	0.9976	0.002392
303.15	0.9970	0.003017
313.15	0.9962	0.003847
322.75	0.9953	0.004693
332.75	0.9943	0.005710
342.85	0.9930	0.006969

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system. Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) Acetophenone; C_8H_8O; [98-86-2]

Original Measurements:
[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.15	0.9993	0.0007249
313.15	0.9991	0.0008585
323.05	0.9989	0.001054
332.95	0.9986	0.001350
342.95	0.9982	0.001748

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system. Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

12.6. 1,3-Benzenedicarboxylic acid solubility data in miscellaneous organic solvents

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]

Original Measurements:
[82]L. Dian-Qing, L. Jiang-Chu, Liu Da-Zhuang, and W. Fu-An, Fluid Phase Equilib. **200**, 69 (2002).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.85	0.8482	0.1518
299.65	0.8477	0.1523
303.55	0.8471	0.1529
309.65	0.8461	0.1539
313.35	0.8454	0.1546
317.25	0.8446	0.1554
322.55	0.8434	0.1566
329.15	0.8419	0.1581
332.55	0.8410	0.1590
337.15	0.8397	0.1603

T/K	x_2[a]	x_1[b]
341.35	0.8383	0.1617
345.75	0.8368	0.1632
349.75	0.8354	0.1646
351.95	0.8346	0.1654
354.55	0.8336	0.1664
357.95	0.8322	0.1678
362.75	0.8301	0.1699
365.05	0.8291	0.1709
370.25	0.8266	0.1734

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) Analytical Reagent, Shanghai Chemical Reagent Company, used as received.
(2) Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]

Original Measurements:
[84]D.-Q. Li, D.-Z. Liu, and F.-A. Wang, J. Chem. Eng. Data **46**, 172 (2001).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.35	0.9107	0.0893
298.85	0.9057	0.0943
303.55	0.8963	0.1037
307.05	0.8885	0.1115
310.25	0.8817	0.1183
313.65	0.8732	0.1268
316.95	0.8654	0.1346
320.45	0.8563	0.1437
323.55	0.8482	0.1518
326.55	0.8392	0.1608
331.25	0.8244	0.1756
336.25	0.8075	0.1925
340.75	0.7905	0.2095
343.55	0.7787	0.2213
345.25	0.7722	0.2278
346.55	0.7660	0.2340

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) 99.5%, Analytical Reagent, Shanghai Chemical Reagent Company, China, used as received.
(2) 99.0%, Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

Components:
(1) 1,3-Benzenedicarboxylic acid; $C_8H_6O_4$; [121-91-5]
(2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]

Original Measurements:
[117]L. Feng, Q. Wang, and X. Li, J. Chem. Eng. Data **53**, 2501 (2008).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
313.2	0.9988	0.001181
323.2	0.9986	0.001436
333.2	0.9982	0.001849
343.2	0.9974	0.002550
353.2	0.9969	0.003145
363.2	0.9958	0.004225

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were reported as grams of solute per kilogram of solvent. Mole fraction solubilities were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium glass bottle, analytical balance, thermoelectric temperature controlling system, and high-performance liquid chromatographic system.
Solubilities were determined using a static method. Excess solute and solvent were sealed in a jacketed equilibrium bottle and allowed to equilibrate for at least 24 h at constant temperature. After equilibrium was obtained, an aliquot of the clear saturated solution was removed by syringe and deposited into a clear test tube that contained about 3 ml of dimethyl sulfoxide. The concentration of the solute was determined by high-performance liquid chromatographic analysis.

Source and Purity of Chemicals:
(1) 99%, Tokyo Kasei Kogyo Company, Ltd., Japan, was used as received.
(2) Purity not given, Hanzhou Chemical Reagent Company, China, was used as received.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

13. Solubility of 1,4-Benzenedicarboxylic Acid in Organic Solvents

13.1. Critical evaluation of experimental solubility data

Several research groups[60,63,80,82,84,91,109,114,115,118–124] have investigated the solubility behavior of 1,4-benzenedicarboxylic acid as a function of temperature. Che *et al.*[109] determined the solubility of 1,4-benzenedicarboxylic acid in tetrahydrofuran, 1,2-diethoxyethane, cyclohexanone, and acetophenone at several temperatures. The internal consistency of the four datasets of measured 1,4-benzenedicarboxylic acid solubilities were assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 19, along with the MRD calculated according to Eq. (24). Examination of the numerical entries in the last column of Table 19 reveals that the largest mean relative deviation between the back-calculated values based on Eq. (8) and experimental data is 2.63%. A significant part of the deviation results from the experimental solubility measurement at 303 K, which is about 10% larger than the calculated value. Results of the mathematical representation analyses indicate that the experimental data for all four 1,4-benzenedicarboxylic acid – organic solvent systems are internally consistent.

Zhao *et al.*[60] measured the solubility of 1,4-benzenedicarboxylic acid in isobutyl ethanoate at ten temperatures between 305 K and 348 K. The experimental data were correlated with the UNIQUAC model. Interaction coefficients calculated from the experimental solid-liquid equilibrium data provided a reasonably accurate mathematical description of the measured values. The mean absolute relative deviation between calculated and observed values was less than 6.5%.

Ma and Xia[80] and Ma and Chen[121] both determined the solubility of 1,4-benzenedicarboxylic acid in *N*,*N*-dimethylformamide, *N*,*N*-dimethylacetamide, and *N*-methyl-2-pyrrolidone. Ma and Xia[80] also performed solubility measurements in ethanoic acid, while Ma and Chen[121] also studied the solubility of 1,4-benzenedicarboxylic acid in dimethyl sulfoxide. Dian-Qing *et al.*[82] conducted solubility measurements in *N*,*N*-dimethylformamide. The internal consistency of the nine datasets was assessed by curve-fitting the measured mole fraction solubility data to the Buchowski λh model [Eq. (9)]. The values of the equation coefficients (λ and h) are given in Table 20, along with the mean relative deviation. The large deviation between observed and back-calculated values noted in the 1,4-benzenedicarboxylic acid–ethanoic acid system is likely due to the extremely small mole fraction solubilities.

Table 19. Parameters of the Modified Apelblat equation for describing the solubility of 1,4-benzenedicarboxylic acid in various organic solvents

Solvent	A	B	C	MRD (%)
1,2-Diethoxyethane[a]	−61.352	1131.2	8.6320	0.46
Tetrahydrofuran[a]	−397.52	16627	−58.757	0.80
Cyclohexanone[a]	−256.51	9662.9	37.813	2.50
Acetophenone[a]	−90.392	−1694.1	14.774	2.63

[a] Values of the coefficients and the mean relative deviations were taken from Che *et al.*[109]

Table 20. Parameters of the Buchowski λh equation for describing the solubility of 1,4-benzenedicarboxylic acid in organic solvents

Solvent	T/K	λ	h	MRD (%)
Ethanoic acid[a]	306–353	0.1448	30 386.1	8.90
N,*N*-Dimethylformamide[a]	293–429	0.0046	16554.7	0.47
N,*N*-Dimethylformamide[b]	296–370	0.0336	11862.9	0.18
N,*N*-Dimethylformamide[c]	298–363	0.1760	5379.87	0.51
N,*N*-Dimethylacetamide[a]	293–365	38.47	122.49	1.15
N,*N*-Dimethylacetamide[c]	293–364	20.06	203.78	1.60
N-Methyl-2-pyrrolidone[a]	298–363	14.13	212.27	1.50
N-Methyl-2-pyrrolidone[c]	296–363	12.94	232.83	1.35
Dimethyl sulfoxide[c]	304–362	0.3166	1926.48	1.35

[a] Values of the coefficients and mean relative deviations were taken from Ma and Xia.[80]

[b] Values of the coefficients and mean relative deviation were taken from Dian-Qing *et al.*[82]

[c] Values of the coefficients and mean relative deviations were taken from Ma and Chen.[121]

Li *et al.*[84] also determined the solubility of 1,4-benzenedicarboxylic acid in *N*-methyl-2-pyrrolidone using a synthetic method with laser monitoring to determine when the last amount of solid solute dissolved. The authors employed a polynomial expression in temperature

$$x_1 = 0.8315 + 0.00602T + 0.09145 \times 10^{-4}\,T^2 + 0.06873 \times 10^{-7}T^3 \quad (38)$$

to represent the measured mole fraction solubility data from 297 to 332 K. The root-mean-square deviation between the observed x_1 data and calculated values from Eq. (38) was on the order of 0.0007 mole fraction. While there is no theoretical basis for this type of polynomial representation in temperature, expressions like Eq. (38) do provide a convenient means for researchers to describe the observed solubility behavior at different temperatures. Wang *et al.*[122] correlated the molar solubility of 1,4-benzenedicarboxylic acid in dimethyl sulfoxide (from 302 to 373 K) and in *N*,*N*-dimethylformamide (from 302 to 373 K) using

$$c_1(\text{in DMSO}) = -59.10 + 0.5414T - 1.648 \times 10^{-3}\,T^2 + 1.714 \times 10^{-6}\,T^3, \quad (39)$$

$$c_1(\text{in DMF}) = -0.2047 + 0.002860T - 0.826 \times 10^{-5}T^2 + 1.740 \times 10^{-8}\,T^3, \quad (40)$$

and similar third-degree polynomial equations.

The experimental solubility data for 1,4-benzenedicarboxylic acid in the different organic solvents are in Secs. 13.2–13.7.

13.2. 1,4-Benzenedicarboxylic acid solubility data in aromatic hydrocarbons

Components:	Original Measurements:
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Methylbenzene; C_7H_8; [108-88-8]	[118]J. J. Harper and P. Janik, J. Chem. Eng. Data **15**, 439 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
485.2	0.9998	0.000230
494.2	0.9997	0.000319
500.2	0.9996	0.000431

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by placing known amounts of solute and solvent into a glass tube, which was then sealed and submerged in a constant-temperature bath. The temperature of the bath was increased at a rate of 1 K/10 min, and the tube was shaken until all of the solute dissolved. The temperature at which all of the solute dissolved was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) 99.8%, Chemical Source not specified, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±5% (relative error).

13.3. 1,4-Benzenedicarboxylic acid solubility data in esters

Components:	Original Measurements:
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Isobutyl ethanoate; $C_6H_{12}O_2$; [110-19-0]	[60]S. Zhao, X. Chen, Q. Dai, and L. Wang, J. Chem. Eng. Data **56**, 2399 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
305.15	0.9999	0.0000238
308.15	0.9999	0.0000257
313.15	0.9999	0.0000322
318.15	0.9999	0.0000341
323.15	0.9999	0.0000386
328.15	0.9999	0.0000578
333.15	0.9999	0.0000707
338.15	0.9999	0.0000825
343.15	0.9999	0.0000891
348.15	0.9999	0.0001043

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated temperature controller, electromagnetic stirrer, analytical balance, an ultraviolet/visible spectrophotometer.
Experimental solubilities were determined by a static method. A sealed flask containing excess solute and solvent was allowed to equilibrate at constant temperature with continuous stirring for 2 h. The stirring was stopped and the excess solid was permitted to settle to the bottom of the flask. Aliquots of the saturated solution were removed, diluted quantitatively with isobutyl ethanoate, and the absorbance recorded at 252 nm. The solubility was calculated based on the Beer-Lambert law using measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.
(2) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.000002.

13.4. 1,4-Benzenedicarboxylic acid solubility data in ethers

Components:	Original Measurements:
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9988	0.0012

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±7.8% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9991	0.0008816
303.15	0.9990	0.0009952
313.45	0.9989	0.001143
323.35	0.9986	0.001398
329.35	0.9984	0.001640

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99%, Kermel Chemical Reagents Development Centre, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9996	0.00042

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±4.5% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[118]J. J. Harper and P. Janik, J. Chem. Eng. Data **15**, 439 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
397.2	0.9966	0.00337
433.7	0.9933	0.00672
471.7	0.9869	0.0131

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by placing known amounts of solute and solvent into a glass tube, which was then sealed and submerged in a constant-temperature bath. The temperature of the bath was increased at a rate of 1 K/10 min, and the tube was shaken until all of the solute dissolved. The temperature at which all of the solute dissolved was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) 99.8%, Chemical source not specified, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±5% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) 1,2-Diethoxyethane; $C_6H_{14}O_2$; [629-14-1]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9998	0.0002137
303.30	0.9997	0.0002513
313.25	0.9997	0.0002936
323.35	0.9997	0.0003439
333.65	0.9996	0.0004034
343.55	0.9995	0.0004770

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system. Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Methoxybenzene; C_7H_8O; [100-66-3]	[118]J. J. Harper and P. Janik, J. Chem. Eng. Data **15**, 439 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
488.2	0.9905	0.00947
513.2	0.9775	0.0225
518.7	0.9732	0.0268

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by placing known amounts of solute and solvent into a glass tube, which was then sealed and submerged in a constant-temperature bath. The temperature of the bath was increased at a rate of 1 K/10 min, and the tube was shaken until all of the solute dissolved. The temperature at which all of the solute dissolved was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) 99.8%, Chemical source not specified, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±5% (relative error).

13.5. 1,4-Benzenedicarboxylic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Methanol; CH_4O; [67-56-1]	[114]G. N. Friedlin and V. N. Davydov, Zh. Prikl. Khim. **35**, 2530 (1962).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

Authors report a solubility of 0.141 g of solute per 100 ml of solvent at 293 K, and a solubility of 0.260 g of solute per 100 ml of solvent at 338 K.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details were not provided.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
Solubility: ±1% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Methanol; CH_4O; [67-56-1]	[115]G. N. Freidlin and V. N. Davydov, Dopov. Akad. Nauk Ukr. RSR 622 (1962).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9997	0.000343
313	0.9996	0.000438
323	0.9995	0.000480
330	0.9995	0.000532
337	0.9994	0.000634

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were expressed as grams of solute per 100 g of solvent. Mole fraction values calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details were not provided.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) 1-Propanol; C_3H_8O; [71-23-8]	[115]G. N. Freidlin and V. N. Davydov, Dopov. Akad. Nauk Ukr. RSR 622 (1962).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9996	0.000401
323	0.9992	0.000813
343	0.9984	0.001571
370	0.9983	0.001734

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were expressed as grams of solute per 100 g of solvent. Mole fraction values calculated by compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details were not provided.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
x_1: ±2% for 293 K value, less than 2% at the other temperatures (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) 2-Propanol; C_3H_8O; [67-63-0]	[91]J. Bradil, J. Malek, and V. Bazant, Chem. Prumysl **20**, 117 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
273.2	0.9998	0.000172
298.2	0.9996	0.000398
323.2	0.9994	0.000561
343.2	0.9992	0.000844

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were reported in terms of grams of dissolved solute per 100 g of solution. Mole fraction solubilities calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent and were placed in a flask and equilibrated at constant temperature with stirring. After 90 min the stirring was discontinued, and the solution was allowed to stand for 30 min to allow the undissolved solid to settle to the bottom of the flask. An aliquot of the saturated solution was removed by pipette fitted with a filtering device. The mass of the aliquot was determined by weighing. The concentration of the dissolved solute was determined by titration using sodium hydroxide, with phenolphthalein being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized in authors' laboratory, prepared from dimethyl-1,4-benzenedicarboxylate.
(2) Purity not given, Lachema, Brono, Czechoslovakia, was distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1% (relative error).

13.6. 1,4-Benzenedicarboxylic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) 3-Pentanone; $C_5H_{10}O$; [99-22-0]	[118]J. J. Harper and P. Janik, J. Chem. Eng. Data **15**, 439 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
417.2	0.9908	0.00919
448.2	0.9822	0.0178
458.7	0.9788	0.0212

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by placing known amounts of solute and solvent into a glass tube, which was then sealed and submerged in a constant-temperature bath. The temperature of the bath was increased at a rate of 1 K/10 min, and the tube was shaken until all of the solute dissolved. The temperature at which all of the solute dissolved was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) 99.8%, Chemical source not specified, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±5% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.15	0.9998	0.0001671
303.15	0.9998	0.0001834
313.15	0.9998	0.0002311
323.30	0.9997	0.0003019
333.40	0.9996	0.0003855
343.85	0.9995	0.0005302

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system. Experimental solubilities were determined by a synthetic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Acetophenone; C_8H_8O; [98-86-2]	[109]Y.-K. Che, Y.-X. Qu, and S. Wang, J. Chem. Eng. Data **54**, 3130 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.15	0.9999	0.0000107
313.15	0.9999	0.0000187
323.15	0.9999	0.0000347
332.85	0.9999	0.0000617
343.30	0.9999	0.0001158

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermostated circulating water bath, electromagnetic stirrer, analytical balance, laser monitoring system. Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99%, Sinopharm Chemical Reagent Company, Ltd., China, no purification details were provided.
(2) 99+%, Tianjin Guangfu Fine Chemical Research Institute, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.5% (relative error).

13.7. 1,4-Benzenedicarboxylic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[80]P. Ma and Q. Xia, Chin. J. Chem. Eng. **9**, 39 (2001).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
305.6	0.9999	0.00003904
310.3	0.9999	0.00004497
315.2	0.9999	0.00005495
319.4	0.9999	0.00006402
325.7	0.9999	0.00008026
329.3	0.9999	0.00008998
334.4	0.9999	0.0001053
339.3	0.9999	0.0001244
343.3	0.9999	0.0001433
348.3	0.9998	0.0001682
355.0	0.9998	0.0002071
357.3	0.9998	0.0002262
363.1	0.9997	0.0002700

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. Near the solid-liquid equilibrium temperature, the rate of temperature increase was 0.1 K/10 min. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[119]M.-M. Chen, P.-S. Ma, L. Wang, and F. Chen, Acta Phys. Chim. Sin. **20**, 445 (2004).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
311.57	0.9999	0.00000470
315.15	0.9999	0.00000670
319.79	0.9999	0.0000110
327.95	0.9999	0.0000229
333.95	0.9999	0.0000402
336.55	0.9999	0.0000512
337.95	0.9999	0.0000582
342.25	0.9999	0.0000864
350.15	0.9999	0.0001370
367.75	0.9997	0.0002569
383.15	0.9996	0.0004287
395.55	0.9994	0.0006344
405.35	0.9992	0.0008559
421.95	0.9986	0.001396
435.75	0.9979	0.002073
444.85	0.9973	0.002673

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell with quartz windows enabling laser monitoring of the inside cell contents, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system.
Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:
(1) 99.95%, Chemical source given only as the factory, no purification details were provided.
(2) 99.9%, Chemical source not given, authors state that ethanoic acid was purified to 99.9%, but no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[120]Q. Wang, H. Xu, and X. Li, J. Chem. Eng. Data **50**, 258 (2005).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
433.2	0.9978	0.00220
443.2	0.9970	0.00296
453.2	0.9963	0.00367
463.2	0.9954	0.00457
473.2	0.9943	0.00571
483.2	0.9929	0.00711
493.2	0.9911	0.00888
503.2	0.9889	0.01105
513.2	0.9862	0.01376

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data are given as grams of dissolved solute per 100 g of solvent. Mole fraction solubilities calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, and a high-performance liquid chromatographic system.
Solubilities were determined using a steady-state method. Excess solute and solvent were sealed in a titanium solid-liquid equilibrium cell and the temperature slowly increased (rate of less than 1 K/min) until the desired temperature was reached. Stirring was continuous during the period of increasing temperature, but was stopped when the experiment temperature was reached in order to allow the suspended particles to settle to the bottom of the container. An aliquot of the saturated solution was removed, and quickly cooled to room temperature to prevent evaporation of the solvent. The concentration of the solute in the sample was determined by a high performance liquid chromatographic method. A more detailed description of experimental apparatus and experimental methodology is given in the paper.

Source and Purity of Chemicals:
(1) 99.5%, Shanghai Chemical Reagent Company, China, no purification details were provided.
(2) 99%, Hangzhou Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N,N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[80]P. Ma and Q. Xia, Chin. J. Chem. Eng. **9**, 39 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.0	0.9737	0.02633
298.1	0.9731	0.02685
304.2	0.9720	0.02803
308.1	0.9714	0.02861
319.0	0.9693	0.03066
329.8	0.9671	0.03293
344.2	0.9660	0.03403
355.3	0.9629	0.03711
359.2	0.9618	0.03818
363.7	0.9612	0.03884
368.8	0.9601	0.03994
376.0	0.9584	0.04156
382.1	0.9570	0.04297
387.0	0.9559	0.04414
393.4	0.9543	0.04571
398.5	0.9530	0.04703
406.6	0.9508	0.04917
413.8	0.9488	0.05115
417.9	0.9477	0.05232
420.4	0.9470	0.05304
423.4	0.9461	0.05392
427.4	0.9449	0.05512
429.3	0.9443	0.05571

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system.
Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. Near the solid-liquid equilibrium temperature, the rate of temperature increase was 0.1 K/10 min. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[121]P. Ma and M. Chen, Chin. J. Chem. Eng. **11**, 334 (2003).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.10	0.9737	0.02629
304.15	0.9716	0.02840
308.10	0.9708	0.02919
312.25	0.9700	0.03001
316.75	0.9679	0.03210
319.04	0.9675	0.03247
321.64	0.9665	0.03352
329.78	0.9643	0.03569
330.35	0.9643	0.03565
340.95	0.9613	0.03872
344.15	0.9600	0.04000
351.15	0.9580	0.04198
354.55	0.9570	0.04301
355.25	0.9567	0.04333
359.15	0.9555	0.04450
360.23	0.9550	0.04497
363.71	0.9536	0.04637

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a solubility cell, and the temperature slowly increased until the solid phase completely disappeared. The rate of temperature increase was 0.1 K/min. The disappearance of the solid solute was observed visually.

Source and Purity of Chemicals:
(1) 99.8%, Chemical source not given, used as received.
(2) 99.5%, Chemical source not given, used as received.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[82]L. Dian-Qing, L. Jiang-Chu, L. Da-Zhuang, and W. Fu-An, Fluid Phase Equilib. **200**, 69 (2002).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.05	0.9722	0.0278
298.85	0.9717	0.0283
301.25	0.9711	0.0289
304.65	0.9704	0.0296
307.35	0.9697	0.0303
311.85	0.9684	0.0316
314.45	0.9680	0.0320
318.05	0.9671	0.0329
320.25	0.9667	0.0333
325.75	0.9652	0.0348
328.25	0.9644	0.0356
331.55	0.9635	0.0365
336.95	0.9621	0.0379
340.25	0.9611	0.0389
343.15	0.9603	0.0397
345.55	0.9596	0.0404
351.65	0.9579	0.0421
353.75	0.9571	0.0429
356.65	0.9562	0.0438
359.95	0.9553	0.0447
365.65	0.9534	0.0466
370.45	0.9517	0.0483

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) Analytical Reagent, Shanghai Chemical Reagent Company, used as received.
(2) Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

Components:

(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0]
(2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]

Original Measurements:

[122]Q. Wang, H. Xu, and X. Li, J. Chem. Eng. Data **50**, 719 (2005).

Variables:

Temperature

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
301.9	0.381
307.5	0.392
315.0	0.418
323.0	0.440
328.6	0.452
334.7	0.474
340.4	0.490
344.2	0.520
351.5	0.539
357.9	0.552
363.6	0.575
369.4	0.611
373.5	0.621

[a] c_1: molar solubility of the solute expressed in units of mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were measured by the static analytical method. Excess solute and solvent were placed in a jacketed glass bottle. The solution was allowed to equilibrate at constant temperature with stirring for several hours. Attainment of equilibrium was verified by repetitive measurements until the results were reproducible to within ±0.5%. Concentration of the dissolved solute was determined by titration with a standardized sodium hydroxide using phenolphthalein as the endpoint indicator.

Source and Purity of Chemicals:

(1) 99.5%, Shanghai Chemical Reagent Company, China, no purification details were provided.
(2) 99+%, Hanzhou Chemical Reagent Company, China, no purification details were provided.

Estimated Error:

Temperature: ±0.1 K.
c_1: ±1% (relative error, estimated by compiler).

Components:

(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0]
(2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:

[80]P. Ma and Q. Xia, Chin. J. Chem. Eng. **9**, 39 (2001).

Variables:

Temperature

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.2	0.9951	0.004914
296.3	0.9942	0.005761
298.5	0.9937	0.006311
303.0	0.9921	0.007914
307.8	0.9904	0.009613
311.5	0.9884	0.01161
320.0	0.9834	0.01663
326.2	0.9779	0.02206
333.7	0.9710	0.02899
340.3	0.9638	0.03622
349.9	0.9501	0.04989
356.3	0.9362	0.06381
362.4	0.9239	0.07614
365.3	0.9116	0.08838

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. Near the solid-liquid equilibrium temperature, the rate of temperature increase was 0.1 K/10 min. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:

(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0]
(2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]

Original Measurements:

[121]P. Ma and M. Chen, Chin. J. Chem. Eng. **11**, 334 (2003).

Variables:

Temperature

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293.19	0.9951	0.004910
296.30	0.9940	0.006000
299.07	0.9933	0.006700
301.76	0.9925	0.007450
305.23	0.9914	0.008590
310.61	0.9894	0.01060
317.42	0.9858	0.01420
326.22	0.9804	0.01960
334.29	0.9730	0.02700
341.70	0.9642	0.03580
348.57	0.9577	0.04230
357.98	0.9412	0.05880
361.75	0.9333	0.06670
364.44	0.9290	0.07100

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a solubility cell, and the temperature slowly increased until the solid phase completely disappeared. The rate of temperature increase was 0.1 K/min. The disappearance of the solid solute was observed visually.

Source and Purity of Chemicals:
(1) 99.8%, Chemical source not given, used as received.
(2) 99.5%, Chemical source not given, used as received.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[123]X. Guo, Y.-W. Cheng, L.-J. Wang, and X. Li, J. Chem. Eng. Data **53**, 1421 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.2	0.9840	0.01597
313.2	0.9789	0.02109
323.2	0.9731	0.02690
333.2	0.9669	0.03311
343.2	0.9615	0.03850
353.2	0.9548	0.04516
363.2	0.9476	0.05237

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance, magnetic stirring system, thermoelectric temperature controlling system, and a high-performance liquid chromatograph.
Excess solute and solvent were placed in a sealed glass bottle and allowed to equilibrate at constant temperature with stirring for 48 h. Attainment of equilibrium was verified by repetitive measurements after an additional 48 h equilibration period and by approaching equilibrium from supersaturation by pre-equilibrating the solutions at a higher temperature. An aliquot of the clear saturated solution was transferred to a volumetric flask and diluted quantitatively with the solvent being studied. The concentration of the diluted solution was determined by high-performance liquid chromatographic analysis.

Source and Purity of Chemicals:
(1) 99.5%, Shanghai Chemical Reagent Company, China, no purification details were provided.
(2) 99.5%, Analytical Reagent grade, Tianjin Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[80]P. Ma and Q. Xia, Chin. J. Chem. Eng. **9**, 39 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.1	0.9673	0.03266
310.4	0.9529	0.04705
314.2	0.9465	0.05347
318.7	0.9387	0.06130
324.9	0.9284	0.07157
331.1	0.9149	0.08510
337.2	0.9018	0.09824
343.3	0.8904	0.1096
349.7	0.8744	0.1256
355.7	0.8522	0.1478
363.7	0.8176	0.1824

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. Near the solid-liquid equilibrium temperature, the rate of temperature increase was 0.1 K/10 min. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[121]P. Ma and M. Chen, Chin. J. Chem. Eng. **11**, 334 (2003).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.60	0.9669	0.03307
302.86	0.9602	0.03977
310.79	0.9513	0.04865
317.54	0.9423	0.05774
325.18	0.9299	0.07011
332.82	0.9149	0.08513
339.35	0.8995	0.1005
346.72	0.8788	0.1212
351.49	0.8632	0.1368
357.76	0.8396	0.1604
363.28	0.8155	0.1845

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a solubility cell, and the temperature slowly increased until the solid phase completely disappeared. The rate of temperature increase was 0.1 K/min. The disappearance of the solid solute was observed visually.

Source and Purity of Chemicals:
(1) 99.8%, Chemical source not given, used as received.
(2) 99.5%, Chemical source not given, used as received.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[84]D.-Q. Li, D.-Z. Liu, and F.-A. Wang, J. Chem. Eng. Data **46**, 172 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.35	0.9699	0.0301
299.55	0.9659	0.0341
303.75	0.9599	0.0401
307.05	0.9549	0.0451
309.75	0.9511	0.0489
312.75	0.9461	0.0539
316.25	0.9395	0.0605
319.65	0.9332	0.0668
324.05	0.9243	0.0757
328.45	0.9151	0.0849
331.55	0.9078	0.0922
332.65	0.9055	0.0945

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) 99.5%, Analytical Reagent, Shanghai Chemical Reagent Company, China, used as received.
(2) 99.0%, Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[123]X. Guo, Y.-W. Cheng, L.-J. Wang, and X. Li, J. Chem. Eng. Data **53**, 1421 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.2	0.9867	0.01334
313.2	0.9845	0.01552
323.2	0.9811	0.01885
333.2	0.9784	0.02165
343.2	0.9744	0.02559
353.2	0.9713	0.02869
363.2	0.9672	0.03276

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance, magnetic stirring system, thermoelectric temperature controlling system, and a high-performance liquid chromatograph.
Excess solute and solvent were placed in a sealed glass bottle and allowed to equilibrate at constant temperature with stirring for 48 h. Attainment of equilibrium was verified by repetitive measurements after an additional 48 h equilibration period and by approaching equilibrium from supersaturation by pre-equilibrating the solutions at a higher temperature. An aliquot of the clear saturated solution was transferred to a volumetric flask and diluted quantitatively with the solvent being studied. The concentration of the diluted solution was determined by high-performance liquid chromatographic analysis.

Source and Purity of Chemicals:
(1) 99.5%, Shanghai Chemical Reagent Company, China, no purification details were provided.
(2) 99.5%, Analytical Reagent grade, Tianjin Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[124]Q. Wang, H. Xu, and X. Li, J. Chem. Eng. Data **50**, 243 (2005).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
343.2	0.9389	0.0611
348.2	0.9311	0.0689
353.2	0.9265	0.0735
358.2	0.9179	0.0821
363.2	0.9134	0.0866
368.2	0.9074	0.0926
373.2	0.9040	0.0960
378.2	0.8958	0.1042
383.2	0.8868	0.1132
388.2	0.8789	0.1211
393.2	0.8657	0.1343
398.2	0.8604	0.1396
403.2	0.8473	0.1527
408.2	0.8326	0.1674
413.2	0.8260	0.1740
418.2	0.8093	0.1907
423.2	0.7970	0.2030
428.2	0.7817	0.2183
433.2	0.7723	0.2277
438.2	0.7509	0.2491
443.2	0.7319	0.2681
448.2	0.7175	0.2825
453.2	0.6963	0.3037
458.2	0.6699	0.3301
463.2	0.6451	0.3549
468.2	0.6180	0.3820

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The numerical values were calculated by the compiler. The solubility data were given in the paper as grams of solute per 100 g of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, and temperature controlling system.
Solubilities were determined using a steady-state method. Excess solute and solvent were placed in a titanium solid-liquid equilibrium cell and allowed to equilibrate at constant temperature. After equilibrium was reached, an aliquot of the saturated solution was removed and filtered through a porous stainless steel filter with an internal aperture size of 1 μm. The mass of the transferred solution was determined by weighing. The solvent was removed by drying *in vacuo* at 323.2 K. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Shanghai Chemical Reagent Company, China, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.5 K.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[122]Q. Wang, H. Xu, and X. Li, J. Chem. Eng. Data **50**, 719 (2005).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
301.9	1.249
307.5	1.330
315.0	1.491
323.0	1.569
328.6	1.650
334.7	1.704
340.4	1.997
344.2	1.876
351.5	1.989
357.9	2.102
363.6	2.244
369.4	2.378
373.5	2.491

[a] c_1: molar solubility of the solute expressed in units of mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were measured by the static analytical method. Excess solute and solvent were placed in a jacketed glass bottle. The solution was allowed to equilibrate at constant temperature with stirring for several hours. Attainment of equilibrium was verified by repetitive measurements until the results were reproducible to within ±0.5%. Concentration of the dissolved solute was determined by titration with a standardized sodium hydroxide using phenolphthalein as the endpoint indicator.

Source and Purity of Chemicals:
(1) 99.5%, Shanghai Chemical Reagent Company, China, no purification details were provided.
(2) 99+%, Hanzhou Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
c_1: ±1% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[121]P. Ma and M. Chen, Chin. J. Chem. Eng. **11**, 334 (2003).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.95	0.9154	0.08459
311.55	0.9069	0.09309
317.78	0.9032	0.09679
325.41	0.8980	0.1020
331.55	0.8958	0.1042
335.52	0.8919	0.1081
341.30	0.8884	0.1116
346.15	0.8863	0.1137
348.64	0.8856	0.1144
354.02	0.8845	0.1155
357.45	0.8834	0.1166
362.49	0.8822	0.1178

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a solubility cell, and the temperature slowly increased until the solid phase completely disappeared. The rate of temperature increase was 0.1 K/min. The disappearance of the solid solute was observed visually.

Source and Purity of Chemicals:
(1) 99.8%, Chemical source not given, used as received.
(2) 99.5%, Chemical source not given, used as received.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 1,4-Benzenedicarboxylic acid; $C_8H_6O_4$; [100-21-0] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[91]J. Bradil, J. Malek, and V. Bazant, Chem. Prumysl **20**, 117 (1970).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
313.2	0.6607	0.3393
333.2	0.5574	0.4426
343.2	0.4340	0.5660

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data were reported in terms of grams of dissolved solute per 100 g of solution. Mole fraction solubilities calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent and were placed in a flask and equilibrated at constant temperature with stirring. After 90 min the stirring was discontinued, and the solution was allowed to stand for 30 min to allow the undissolved solid to settle to the bottom of the flask. An aliquot of the saturated solution was removed by a pipette fitted with a filtering device. The mass of the aliquot was determined by weighing. The concentration of the dissolved solute was determined by titration using sodium hydroxide, with phenolphthalein being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized in authors' laboratory, prepared from dimethyl-1,4-benzenedicarboxylate.
(2) Purity not given, Sojuz Chemical Export, Moscow, Soviet Union, mixed with activated carbon and distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1% (relative error).

14. Solubility of 1,3,5-Benzenetricarboxylic Acid in Organic Solvents

14.1. Critical evaluation of experimental solubility data

There is only a single published study regarding the solubility behavior of 1,3,5-benzenetricarboxylic acid in organic solvents. Feng *et al.*[117] determined the solubility of 1,3,5-benzenetricarboxylic acid in ethanoic acid in the temperature range of 313–363 K. The calculated curve-fit parameters from the Buchowski λh-model [Eq. (9)] of $\lambda = 0.0170$ and $h = 131653.7$ described the observed solubility data to within a mean relative deviation of 2.9%.

The experimental solubility data for 1,3,5-benzenetricarboxylic acid in ethanoic acid are given in Sec. 14.2.

14.2. 1,3,5-Benzenetricarboxylic acid solubility data in miscellaneous organic solvents

Components:	Original Measurements:
(1) 1,3,5-Benzenetricarboxylic acid; $C_9H_6O_6$; [554-95-0] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[117]L. Feng, Q. Wang, and X. Li, J. Chem. Eng. Data **53**, 2501 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
313.2	0.9988	0.001200
323.2	0.9987	0.001340
333.2	0.9983	0.001691
343.2	0.9980	0.002000
353.2	0.9975	0.002489
363.2	0.9968	0.003173

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data were reported as grams of dissolved solute per kilogram of solvent. Mole fraction solubilities were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed equilibrium glass bottle, analytical balance, thermoelectric temperature controlling system, and high-performance liquid chromatographic system.

Solubilities were determined using a static method. Excess solute and solvent were sealed in a jacketed equilibrium bottle and allowed to equilibrate for at least 24 h at constant temperature. After equilibrium was obtained, an aliquot of the clear saturated solution was removed by syringe and deposited into a clear test tube that contained about 3 ml of dimethyl sulfoxide. The concentration of the solute was determined by high-performance liquid chromatographic analysis.

Source and Purity of Chemicals:

(1) 98%, Alfa Aesar, used as received.

(2) Purity not given, Hanzhou Chemical Reagent Company, China, used as received.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

x_1: ±3% (relative error, estimated by compiler).

15. Solubility of 2-Bromobenzoic Acid in Organic Solvents

15.1. Critical evaluation of experimental solubility data

There have been only two publications[72,125] reporting the solubility of 2-bromobenzoic acid in organic solvents. Thuaire[72] determined the solubility of 2-bromobenzoic acid in ethanol at 298 K as part of study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. Pinsuwan *et al.*[125] measured the solubility of 2-bromobenzoic acid in 1-octanol to examine correlations between experimental octanol/water solubility ratios and measured water-to-1-octanol practical partition coefficients. It is not possible to perform a critical evaluation of the experimental data as measurements were made at only a single temperature, and there are no independent experimental 2-bromobenzoic acid solubility data in either ethanol or 1-octanol.

The experimental solubility data for 2-bromobenzoic acid in organic solvents are given in Sec. 15.2.

15.2. 2-Bromobenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 2-Bromobenzoic acid; $C_7H_5BrO_2$; [88-65-3] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 3.250 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1302$

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: ±0.05 K.

x_1: ±4% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Bromobenzoic acid; $C_7H_5BrO_2$; [88-65-3] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[125]S. Pinsuwan, A. Li, and S. H. Yalkowsky, J. Chem. Eng. Data **40**, 623 (1995).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $\log_{10} c_1 = -0.12$, which corresponds to a molar solubility of $c_1 = 0.759$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, mechanical stirrer, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated at (298 ± 2) K in a sealed vial for 48–72 h. The solution was mixed using an end-over-end mechanical stirrer. After equilibrium was obtained, the saturated sample was vacuum filtered through a 5.0 μm fritted glass filter. An aliquot of the filtrate was diluted quantitatively with 2-propanol, and the absorbance of the diluted sample was recorded. The solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) Purity not given, Chemical source not given, used as received.

Estimated Error:
Temperature: ±2 K.
c_1: ±10% (relative error, estimated by compiler given the large uncertainty in temperature).

16. Solubility of 3-Bromobenzoic Acid in Organic Solvents

16.1. Critical evaluation of experimental solubility data

There have been several publications[54,63,72,76,83,125] reporting the solubility of 3-bromobenzoic acid in organic solvents. Chantooni and Kolthoff[83] determined the solubility of 3-bromobenzoic acid in methanol and ethanenitrile at 298 K. In a followup study,[76] the authors extended their measurements to include 2-propanol, 2-methyl-2-propanol, and 1-hexanol. Hancock *et al.*[54,63] measured the solubility of 3-bromobenzoic acid in cyclohexane, benzene, tetrahydrofuran, and 1,4-dioxane at 303 K based on a gravimetric method. Thuaire[72] determined the solubility of 3-bromobenzoic acid in ethanol at 298 K as part of study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. Pinsuwan *et al.*[125] measured the solubility of 3-bromobenzoic acid in 1-octanol to examine correlations between experimental octanol/water solubility ratios and measured water-to-1-octanol practical partition coefficients. It is not possible to perform a critical evaluation of the experimental data as each of the research groups performed measurements at only a single temperature, and there are no independent experimental 3-bromobenzoic acid solubility data in any of the 11 aforementioned organic solvents.

The experimental solubility data for 3-bromobenzoic acid in organic solvents are given in Secs. 16.2–16.6.

16.2. 3-Bromobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9984	0.00160

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

16.3. 3-Bromobenzoic acid solubility data in aromatic hydrocarbons

Components:	Original Measurements:
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9898	0.0102

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

16.4. 3-Bromobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.751	0.249

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.817	0.183

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

16.5. 3-Bromobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.51 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from acetone and dried *in vacuo* at 343 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.955 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.0826$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) 2-Propanol; C_3H_8O; [67-63-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.20 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from acetone and dried *in vacuo* at 343 K.
(2) No Purity given, Fisher Scientific, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.35 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from acetone and dried *in vacuo* at 343 K.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.99 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from acetone and dried *in vacuo* at 343 K.
(2) Yellow Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[125]S. Pinsuwan, A. Li, and S. H. Yalkowsky, J. Chem. Eng. Data **40**, 623 (1995).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $\log_{10} c_1 = -0.07$, which corresponds to a molar solubility of $c_1 = 0.851$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, mechanical stirrer, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated at (298 ± 2) K in a sealed vial for 48 to 72 h. The solution was mixed using an end-over-end mechanical stirrer. After equilibrium was obtained, the saturated sample was vacuum filtered through a 5.0 μm fritted glass filter. An aliquot of the filtrate was diluted quantitatively with 2-propanol, and the absorbance of the diluted sample was recorded. The solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) Purity not given, Chemical source not given, used as received.

Estimated Error:
Temperature: ±2 K.
c_1: ±10% (relative error, estimated by compiler given the large uncertainty in temperature).

16.6. 3-Bromobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3-Bromobenzoic acid; $C_7H_5BrO_2$; [585-76-2] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.167 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson,

J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from acetone and dried *in vacuo* at 343 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

17. Solubility of 4-Bromobenzoic Acid in Organic Solvents

17.1. Critical evaluation of experimental solubility data

There have been several publications[54,72,76,83,125] reporting the solubility of 4-bromobenzoic acid in organic solvents. Chantooni and Kolthoff[83] determined the solubility of 4-bromobenzoic acid in methanol, ethanenitrile, dimethyl sulfoxide, and *N*,*N*-dimethylformamide at 298 K. In a followup study, the authors[76] extended their measurements to include 2-propanol, 2-methyl-2-propanol, and 1-hexanol. Hancock *et al.*[54] measured the solubility of 4-bromobenzoic acid in cyclohexane and benzene at 303 K based on a gravimetric method. Thuaire[72] determined the solubility of 4-bromobenzoic acid in ethanol at 298 K as part of a study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. Pinsuwan *et al.*[125] measured the solubility of 4-bromobenzoic acid in 1-octanol to examine correlations between experimental octanol/water solubility ratios and measured water-to-1-octanol practical partition coefficients. It is not possible to perform a critical evaluation of the experimental data as each of the research groups performed measurements at only a single temperature, and there are no independent experimental 4-bromobenzoic acid solubility data in any of the 11 organic solvents.

The experimental solubility data for 4-bromobenzoic acid in organic solvents are given in Secs. 17.2–17.5.

17.2. 4-Bromobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000362

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

17.3. 4-Bromobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9997	0.000272

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±5% (relative error, by compiler).

17.4. 4-Bromobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.12 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.164 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.00750$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) 2-Propanol; C_3H_8O; [67-63-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.112 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson,

J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) No Purity given, Fisher Scientific, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15 K	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.125 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.103 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Yellow Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[125]S. Pinsuwan, A. Li, and S. H. Yalkowsky, J. Chem. Eng. Data **40**, 623 (1995).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $\log_{10} c_1 = -1.11$, which corresponds to a molar solubility of $c_1 = 0.0776$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, mechanical stirrer, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated at (298 ± 2) K in a sealed vial for 48 to 72 h. The solution was mixed using an end-over-end mechanical stirrer. After equilibrium was obtained, the saturated sample was vacuum filtered through a 5.0 μm fritted glass filter. An aliquot of the filtrate was diluted quantitatively with 2-propanol, and the absorbance of the diluted sample was recorded. The solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, used as received.
(2) Purity not given, Chemical source not given, used as received.

Estimated Error:
Temperature: ±2 K.
c_1: ±10% (relative error, estimated by compiler given the large uncertainty in temperature).

17.5. 4-Bromobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.018 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.45 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was shaken with activated alumina and then distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Bromobenzoic acid; $C_7H_5BrO_2$; [586-76-5] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.93 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

18. Solubility of 2-Chlorobenzoic Acid in Organic Solvents

18.1. Critical evaluation of experimental solubility data

There have been several published studies[54,72,83,99,126,127] investigating the solubility behavior of 2-chlorobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Chantooni and Kolthoff[83] determined the solubility of 2-chlorobenzoic acid in methanol, ethanenitrile, and *N*,*N*-dimethylformamide at 298 K. Hancock *et al.*[54] measured the solubility of 2-chlorobenzoic acid in cyclohexane and benzene at 303 K based on a gravimetric method. Thuaire[72] determined the solubility of 2-chlorobenzoic acid in ethanol at 298 K as part of study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. Biswas *et al.*[126] also measured the solubility of 2-chlorobenzoic acid in ethanol at 298 K. The two independent experimental determinations of the mole fraction solubility of 2-chlorobenzoic acid in ethanol differ significantly from one another, $x_1 = 0.0708$ (Biswas value, Ref. 126) versus $x_1 = 0.1424$ (Thuaire value, Ref. 72). Given only two independent measurements it is normally impossible to know of the two values is best. However, in the present case, both research groups have performed independent experimental measurements for other substituted benzoic acid derivatives in ethanol. For several of the other solutes (e.g., 3-chlorobenzoic acid, 4-chlorobenzoic acid, and 4-nitrobenzoic acid), there does exist at least one additional set of observed values. One finds that the measured values reported by Thuaire[72] are in better agreement with experimental data reported by other research groups than are the observed values reported by Biswas *et al.*[126]

Sidgwick and Ewbank[127] measured the solubility of 2-chlorobenzoic acid in heptane and benzene as a function of temperature. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model to yield the following two representations:

$$\ln x_1 = -167.18 + \frac{112.27}{T} + 27.681 \ln T, \tag{41}$$

$$\ln x_1 = -93.217 + \frac{113.76}{T} + 15.491 \ln T, \tag{42}$$

for solubilities in heptane and benzene, respectively. The average absolute deviations between the observed experimental data and back-calculated values based on Eqs. (41) and (42) of 26.1% and 8.3% are larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0166$ to $x_1 = 0.834$ for heptane and $x_1 = 0.0100$ to $x_1 = 0.833$ for benzene. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

Jia *et al.*[99] determined the solubility of 2-chlorobenzoic acid in 1-octanol in the temperature range of 293–323 K. The calculated curve-fit parameters from the Buchowski λh-model [Eq. (9)] of $\lambda = 1.885$ and $h = 1567.8$ described the observed solubility data to within a mean relative deviation of 1.7%.

The experimental solubility data for 2-chlorobenzoic acid in organic solvents are in Secs. 18.2–18.5.

18.2. 2-Chlorobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) Heptane; C_7H_{16}; [142-82-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
352.2	0.983	0.0166
368.0	0.970	0.0300
382.0	0.931	0.0693
386.0	0.916	0.0841
399.2	0.728	0.272
401.2	0.591	0.409
403.0	0.415	0.585
407.9	0.166	0.834

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 413.5 K.
(2) Purity not given, sample isolated from the resin of *Pinus sabiniana*, purified by treatment with sulfuric acid and nitric acid, and then distilled before use.

Estimated Error:

Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

18.3. 2-Chlorobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
299.2	0.990	0.0100
318.0	0.974	0.0264
330.9	0.948	0.0520
355.9	0.825	0.175
372.8	0.666	0.334
387.1	0.457	0.543
402.7	0.167	0.833

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 413.5 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

18.4. 2-Chlorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.53 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) Ethanol; C_2H_6O; [64-17-5]	[126]P. K. Biswas, S. C. Lahiri, and B. P. Dey, Bull. Chem. Soc. Jpn. **66**, 2785 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
1.1275	0.9292	0.0708

[a] c_1: solubility of the solute expressed in units of mol dm^{-3}.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and an ultraviolet/visible spectrophotometer.
Solutions containing excess solute and solvent were allowed to equilibrate at constant temperature for at least 24 h. An aliquot of the saturated solution was removed, filtered, and the absorbance recorded. Solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Puris grade, Fluka Chemicals, recrystallized from aqueous ethanol mixture and dried in an air oven at 390 K. The purified compound was stored in vacuum desiccators.
(2) Absolute, B.C.P.W., Calcutta, India, was distilled twice before use.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±1.0% (relative error, estimated by compiler).
x_1: ±2.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 3.607 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1424$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[99]Q. Jia, P. Ma, S. Ma, and C. Wang, Chin. J. Chem. Eng. **15**, 710 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.65	0.8914	0.1086
298.55	0.8877	0.1123
298.90	0.8864	0.1136
299.10	0.8856	0.1144
304.75	0.8602	0.1398
306.40	0.8527	0.1473
308.00	0.8454	0.1546
309.55	0.8380	0.1620
311.15	0.8309	0.1691
313.05	0.8240	0.1760
315.10	0.8172	0.1828
316.70	0.8103	0.1897
318.65	0.8035	0.1965
319.95	0.7994	0.2006

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature circulating bath, stirrer, analytical balance, and laser monitoring system.
Solubilities were determined by a dynamic method. Preweighed amounts of solute and solvent were placed in a stoppered equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and the temperature slowly increased until all of the solid dissolved. Near the dissolution temperature, the temperature was increased at a rate of 0.2 K/20 min. Complete dissolution was determined using a laser monitoring system.

Source and Purity of Chemicals:
(1) 99+%, Chemical source not specified, no purification details were provided.
(2) 99+%, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

18.5. 2-Chlorobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
$T/K = 298.15$	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.53 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Chlorobenzoic acid; $C_7H_5ClO_2$; [118-91-2] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
$T/K = 298.15$	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 4.74 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K
(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

19. Solubility of 3-Chlorobenzoic Acid in Organic Solvents

19.1. Critical evaluation of experimental solubility data

There have been several published studies[8,18,54,61,72,126,127] investigating the solubility behavior of 3-chlorobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Hoover *et al.*[8] measured the solubility of 3-chlorobenzoic acid in 11 alcohols (1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 1-pentanol, 3-methyl-1-butanol, 1-hexanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and one cyclic ether (tetrahydrofuran), and in three alkyl alkanoates (ethyl ethanoate, butyl ethanoate, and pentyl ethanoate) at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 3-chlorobenzoic acid. The authors were able to assemble a total of 37 $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) equations for which experimental partition coefficient data, solubility ratios, Abraham Model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 3-chlorobenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -2.65$.[72] The McGowan volume of 3-chlorobenzoic acid, $V = 1.0541$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.840$. This left four solute descriptors (S, A, B and L) still to be determined. The 37 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 0.950$, $A = 0.630$, $B = 0.320$, and $L = 5.197$, that best described the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -7.80$ for the logarithm of the gas-phase solute concentration that made the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values to within an average standard deviation of 0.081 and 0.088 $\log_{10}$ units, respectively.

TABLE 21. Comparison between observed and calculated molar solubilities of 3-chlorobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Ethanol	0.073[a]	0.105	0.077
1-Propanol	0.042[b]	0.003	−0.001
2-Propanol	0.054[b]	0.024	−0.032
1-Butanol	−0.009[b]	−0.077	−0.073
2-Butanol	−0.018[b]	−0.044	−0.071
2-Methyl-1-propanol	−0.135[b]	−0.165	−0.196
1-Pentanol	−0.035[b]	−0.067	−0.064
3-Methyl-1-butanol	−0.098[b]	−0.129	−0.142
1-Hexanol	−0.069[b]	−0.112	−0.121
1-Heptanol	−0.127[b]	−0.128	−0.140
1-Octanol	−0.146[b]	−0.189	−0.244
1-Decanol	−0.220[b]	−0.246	−0.230
1,1′-Oxybisethane	−0.121[b]	−0.149	−0.009
Tetrahydrofuran	0.400[b]	0.476	0.463
1,4-Dioxane	0.215[c]	0.160	0.152
Ethyl ethanoate	−0.185[b]	−0.072	−0.082
Butyl ethanoate	−0.298[b]	−0.204	−0.239

[a] Experimental value is from the study of Thuaire.[72]
[b] Experimental values are from Hoover *et al.*[8]
[c] Experimental value is from the study of Saifullah *et al.*[18]

After the 3-chlorobenzoic acid solubility study was published, Abraham model correlations have been developed for 3-methyl-1-butanol and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 3-chlorobenzoic acid solubility data. Table 21 compares the experimental $\log_{10}$ c_1 values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 3-chlorobenzoic acid, x_1, determined by Hoover *et al.*[8] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 3-chlorobenzoic acid is $V_{\mathrm{solute}} = 117.08$ cm^3 mol^{-1}. Examination of the numerical entries in Table 21 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Sidgwick and Ewbank[127] measured the solubility of 3-chlorobenzoic acid in heptane and benzene as a function of temperature. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model to yield the following two representations:

$$\ln x_1 = -133.498 + \frac{112.89}{T} + 22.0061\ \ln T, \qquad (43)$$

$$\ln x_1 = -91.101 + \frac{113.72}{T} + 15.0631\ \ln T, \qquad (44)$$

for solubilities in heptane and benzene, respectively. The average absolute deviations between the observed experimental data and back-calculated values based on Eqs. (43) and (44) of 12.8% and 9.4% are larger than desired. The large deviations may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0124$ to $x_1 = 0.850$ for heptane and $x_1 = 0.0114$ to $x_1 = 0.821$ for benzene. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 3-chlorobenzoic acid in organic solvents are in Secs. 19.2–19.6.

19.2. 3-Chlorobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Heptane; C_7H_{16}; [142-82-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
345.4	0.988	0.0124
362.8	0.971	0.0291
379.0	0.934	0.0663
401.3	0.780	0.220
407.4	0.609	0.391
413.3	0.400	0.600
420.9	0.150	0.850

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 427.7 K.
(2) Purity not given, sample isolated from the resin of *Pinus sabiniana*, purified by treatment with sulfuric acid and nitric acid, and then distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9985	0.00145

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

19.3. 3-Chlorobenzoic acid solubility data in aromatic hydrocarbons

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9905	0.00948

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
309.0	0.989	0.0114
324.4	0.975	0.0254
338.7	0.949	0.0507
366.9	0.823	0.177
381.2	0.676	0.324
398.5	0.448	0.552
415.7	0.179	0.821

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 427.7 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

19.4. 3-Chlorobenzoic acid solubility data in esters

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9348	0.0652

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9338	0.0662

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9368	0.0632

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Methylethyl tetradecanoate; $C_{17}H_{34}O_2$; [110-27-0]	[61]E. R. Cooper, J. Control. Release **1**, 153 (1984).
Variables: T/K = 295	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.956	0.044

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Aldrich Chemical Company, Metuchen, NJ, USA, no purification details provided.
(2) Reagent grade, Wickhen Corporation, Huguenot, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9458	0.05424

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

19.5. 3-Chlorobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9199	0.0801

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9449	0.0551

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9621	0.0379

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7755	0.2245

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[18]M. Saifullah, S. Ye, L. M. Grubbs, N. E. De La Rosa, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **40**, 2082 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8515	0.1485

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

19.6. 3-Chlorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Ethanol; C_2H_6O; [64-17-5]	[126]P. K. Biswas, S. C. Lahiri, and B. P. Dey, Bull. Chem. Soc. Jpn. **66**, 2785 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.6480	0.9605	0.0395

[a] c_1: solubility of the solute expressed in units of mol dm^{-3}.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and an ultraviolet/visible spectrophotometer.
Solutions containing excess solute and solvent were allowed to equilibrate at constant temperature for at least 24 h. An aliquot of the saturated solution was removed, filtered, and the absorbance recorded. Solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Puris grade, Fluka Chemicals, recrystallized from aqueous ethanol mixture and dried in an air oven at 390 K. The purified compound was stored in vacuum desiccators.
(2) Absolute, B.C.P.W., Calcutta, India, was distilled twice before use.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±1.0% (relative error, estimated by compiler).
x_1: ±2.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.750 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.0746$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Propanol; C_3H_8O; [71-23-8]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9133	0.0867

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 2-Propanol; C_3H_8O; [67-63-0]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9087	0.0913

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9075	0.0925

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9093	0.0907

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9308	0.0692

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8990	0.1010

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 3-Methyl-1-butanol; $C_5H_{10}O$; [123-51-3]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9118	0.0882

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8940	0.1060

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8961	0.1039

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8901	0.1099

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[8]K. R. Hoover, K. Pop, W. E. Acree, Jr., and M. H. Abraham, S. Afr. J. Chem. **58**, 25 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8896	0.1104

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Chlorobenzoic acid; $C_7H_5ClO_2$; [535-80-8] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[61]E. R. Cooper, J. Control. Release **1**, 153 (1984).
Variables:	**Prepared by:**
T/K = 295	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.949	0.051

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Aldrich Chemical Company, Metuchen, NJ, USA, no purification details provided.
(2) Reagent grade, J.T. Baker Chemical Company, Phillipsburg, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

20. Solubility of 4-Chlorobenzoic Acid in Organic Solvents

20.1. Critical evaluation of experimental solubility data

There have been several published studies[14,54,61,127–130] investigating the solubility behavior of 4-chlorobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Daniels *et al.*[14] measured the solubility of 4-chlorobenzoic acid in 16 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 1-hexanol, 1-heptanol, 1-octanol, and 1-decanol), in two dialkyl ethers (2,2′-oxybispropane and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in three alkanoates (methyl ethanoate, ethyl ethanoate, and butyl ethanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 4-chlorobenzoic acid. The authors were able to assemble a total of 49 $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 4-chlorobenzoic acid is $\log_{10} c_{1,W} = -3.56$.[131–135] The McGowan volume of 4-chlorobenzoic acid, $V = 1.0541$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.840$. This left four solute descriptors (S, A, B, and L) still to be determined. The 49 equations were then solved using the Microsoft “SOLVER” program to yield numerical values of the remaining four solute descriptors, $S = 1.020$, $A = 0.630$, $B = 0.270$, and $L = 4.9474$, that best described the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values. The computation treated $\log_{10} c_{1,G}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,G} = -8.360$ for the gas-phase solute concentration that made the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values to

TABLE 22. Comparison between observed and calculated molar solubilities of 4-chlorobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\text{exp},a}$	$\log_{10} c_1^{\text{calc}}$; Eq. (20)	$\log_{10} c_1^{\text{calc}}$; Eq. (21)
Methanol	−0.701	−0.734	−0.728
Ethanol	−0.767	−0.698	−0.693
1-Propanol	−0.800	−0.790	−0.781
2-Propanol	−0.780	−0.768	−0.752
1-Butanol	−0.840	−0.860	−0.845
2-Butanol	−0.800	−0.828	−0.861
2-Methyl-1-propanol	−0.990	−0.976	−0.990
2-Methyl-2-propanol	−0.670	−0.734	−0.704
1-Pentanol	−0.860	−0.870	−0.860
2-Pentanol	−0.821	−0.874	−0.872
3-Methyl-1-butanol	−0.919	−0.940	−0.939
1-Hexanol	−0.880	−0.905	−0.913
1-Heptanol	−0.900	−0.895	−0.934
1-Octanol	−0.920	−0.960	−1.038
1-Decanol	−0.988	−1.040	−1.041
Tetrahydrofuran	−0.153	−0.215	−0.258
1,4-Dioxane	−0.465	−0.512	−0.518
Methyl ethanoate	−0.951	−0.862	−0.822
Ethyl ethanoate	−0.950	−0.768	−0.780
Butyl ethanoate	−1.155	−0.900	−0.952

[a] All experimental data were taken from Daniels *et al.*[14]

within an average standard deviation of 0.078 and 0.098 $\log_{10}$ units, respectively.

After the 4-chlorobenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, methyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 4-chlorobenzoic acid solubility data. Table 22 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 4-chlorobenzoic acid, x_1, determined by Daniel *et al.*[14] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\text{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\text{solvent}}]$). The molar volume of the hypothetical subcooled liquid 4-chlorobenzoic acid is $V_{\text{solute}} = 117.08\ \text{cm}^3\ \text{mol}^{-1}$. Examination of the numerical entries in Table 22 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Sidgwick and Ewbank[127] measured the solubility of 4-chlorobenzoic acid in heptane and benzene as a function of temperature. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model to yield the following representations:

$$\ln x_1 = -130.159 + \frac{113.10}{T} + 20.8141 \ln T, \qquad (45)$$

$$\ln x_1 = -89.694 + \frac{113.78}{T} + 14.3691 \ln T, \qquad (46)$$

for solubilities in heptane and benzene, respectively. The average absolute deviations between the observed experimental data and back-calculated values based on Eqs. (45) and (46) of 12.4% and 6.7% are larger than desired. The large deviations may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0109$ to $x_1 = 0.680$ for heptane and $x_1 = 0.0100$ to $x_1 = 0.855$ for benzene. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 4-chlorobenzoic acid in organic solvents are in Secs. 20.2–20.9.

20.2. 4-Chlorobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Heptane; C_7H_{16}; [142-82-5]	[127] N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
409.3	0.989	0.0109
438.5	0.968	0.0323
454.1	0.933	0.0670
480.4	0.775	0.225
491.5	0.597	0.403
500.8	0.320	0.680

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 514.7 K.
(2) Purity not given, sample isolated from the resin of *Pinus sabiniana*, purified by treatment with sulfuric acid and nitric acid, and then distilled before use.

Estimated Error:

Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000719

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.1 g/l, which corresponds to a molar solubility of $c_1 = 0.00064$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

20.3. 4-Chlorobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9995	0.000489

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error, by compiler).

Components:	Original Measurements:
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
366.8	0.990	0.0100
392.6	0.973	0.0272
410.6	0.946	0.0542
445.7	0.820	0.1796
467.2	0.645	0.355
485.9	0.427	0.573
505.7	0.145	0.855

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 514.7 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Benzene; C_6H_6; [71-43-2]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.5 g/l, which corresponds to a molar solubility of $c_1 = 0.0032$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

20.4. 4-Chlorobenzoic acid solubility data in esters

Components:	Original Measurements:
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9910	0.008963

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9889	0.01111

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9907	0.00926

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Methylethyl tetradecanoate; $C_{17}H_{34}O_2$; [110-27-0]	[61]E. R. Cooper, J. Control. Release **1**, 153 (1984).
Variables:	**Prepared by:**
T/K = 295	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9914	0.0086

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Aldrich Chemical Company, Metuchen, NJ, USA, no purification details provided.
(2) Reagent grade, Wickhen Corporation, Huguenot, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9894	0.01060

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

20.5. 4-Chlorobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables: T/K = 293	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 15.2 g/l, which corresponds to a molar solubility of $c_1 = 0.097$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9932	0.006780

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9942	0.005833

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,2-Dimethoxyethane; $C_4H_{10}O_2$; [110-71-4]	[129]S. H. Ghosh and D. K. Hazra, J. Ind. Chem. Soc. **65**, 620 (1988).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $c_1 = 1.0369$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Mechanical shaker and a constant-temperature thermostat.
Excess solute and solvent were placed in a bottle and stoppered. The solution was shaken in a mechanical shaker for 24 h at ambient room temperature. The solution was then thermostated at 298 K for 24 h with occasional shaking. An aliquot of the saturated solution was then removed and filtered. The concentration of the dissolved solute was determined by titration with standard caustic soda using phenolphthalein as indicator.

Source and Purity of Chemicals:
(1) Puriss, Fluka, distilled from aqueous-ethanol mixture.
(2) Purum, Fluka, was shaken with ferrous sulfate and then distilled. The distillate was further purified by refluxing for 12 h and distilling over metallic sodium.

Estimated Error:
Temperature: ±0.01 K.
c_1: ±1.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9413	0.05874

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9703	0.02974

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 53.0 g/l, which corresponds to a molar solubility of $c_1 = 0.339$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

20.6. 4-Chlorobenzoic acid solubility in haloalkanes, haloalkenes, haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.1 g/l, which corresponds to a molar solubility of $c_1 = 0.0134$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Tetrachloromethane; CCl_4; [56-23-5]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.2 g/l, which corresponds to a molar solubility of $c_1 = 0.0013$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.4 g/l, which corresponds to a molar solubility of $c_1 = 0.0089$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.4 g/l, which corresponds to a molar solubility of $c_1 = 0.0089$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.7 g/l, which corresponds to a molar solubility of $c_1 = 0.0045$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

20.7. 4-Chlorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Methanol; CH_4O; [67-56-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9918	0.00823

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Ethanol; C_2H_6O; [64-17-5]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9899	0.01013

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Ethanol; C_2H_6O; [64-17-5]	[126]P. K. Biswas, S. C. Lahiri, and B. P. Dey, Bull. Chem. Soc. Jpn. **66**, 2785 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.2895	0.9827	0.0173

[a] c_1: solubility of the solute expressed in units of mol dm^{-3}.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and an ultraviolet/visible spectrophotometer.
Solutions containing excess solute and solvent were allowed to equilibrate at constant temperature for at least 24 h. An aliquot of the saturated solution was removed, filtered, and the absorbance recorded. Solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Puris grade, Fluka Chemicals, recrystallized from aqueous ethanol mixture and dried in an air oven at 390 K. The purified compound was stored in vacuum desiccators.
(2) Absolute, B.C.P.W., Calcutta, India, was distilled twice before use.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±1.0% (relative error, estimated by compiler).
x_1: ±2.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.270 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.01229$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Ethanol; C_2H_6O; [64-17-5]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 25.5 g/l, which corresponds to a molar solubility of $c_1 = 0.163$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Propanol; C_3H_8O; [71-23-8]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9881	0.01188

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Propanol; C_3H_8O; [71-23-8]	[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).
Variables:	**Prepared by:**
T/K = 293	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 23.8 g/l, which corresponds to a molar solubility of $c_1 = 0.152$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Propanol; C_3H_8O; [71-23-8]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9873	0.01274

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9865	0.01350

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9852	0.01480

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9904	0.009578

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3]
(2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]

Original Measurements:
[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9798	0.02021

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3]
(2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]

Original Measurements:
[128]G. S. Krasil'nikova, E. G. Freidlin, and Y. N. Pirig, Zh. Prikl. Khim. **60**, 2519 (1987).

Variables:
T/K = 293

Prepared by:
W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 30.7 g/l, which corresponds to a molar solubility of $c_1 = 0.196$.

Auxiliary Information

Method/Apparatus/Procedure:
No information given.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information given.
c_1: No information given.

Components:
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3]
(2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]

Original Measurements:
[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9848	0.01517

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3]
(2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]

Original Measurements:
[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9835	0.01655

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9887	0.01133

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9868	0.01323

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9835	0.01646

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9822	0.01777

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9811	0.01885

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9804	0.01956

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[61]E. R. Cooper, J. Control. Release **1**, 153 (1984).
Variables: T/K = 295	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[cb]
0.9902	0.0098

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Aldrich Chemical Company, Metuchen, NJ, USA, no purification details provided.
(2) Reagent grade, J.T. Baker Chemical Company, Phillipsburg, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

20.8. 4-Chlorobenzoic acid solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[129]S. H. Ghosh and D. K. Hazra, J. Indian Chem. Soc. **65**, 620 (1988).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $c_1 = 0.4031$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Mechanical shaker and a constant-temperature thermostat.
Excess solute and solvent were placed in a bottle and stoppered. The solution was shaken in a mechanical shaker for 24 h at ambient room temperature. The solution was then thermostated at 298 K for 24 h with occasional shaking. An aliquot of the saturated solution was then removed and filtered. The concentration of the dissolved solute was determined by titration with standard caustic soda using phenolphthalein as indicator.

Source and Purity of Chemicals:
(1) Puriss, Fluka, distilled from aqueous-ethanol mixture.
(2) G. R., Merck Chemical Company, was distilled twice before use.

Estimated Error:
Temperature: ±0.01 K.
c_1: ±1.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9663	0.0337

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9691	0.0309

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9646	0.0354

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9701	0.0299

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

20.9. 4-Chlorobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Chlorobenzoic acid; $C_7H_5ClO_2$; [74-11-3] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9967	0.003247

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

21. Solubility of 2-Chloro-5-nitrobenzoic Acid in Organic Solvents

21.1. Critical evaluation of experimental solubility data

There has been only one published study investigating the solubility behavior of 2-chloro-5-nitrobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Stovall *et al.*[13] measured the solubility of 2-chloro-5-nitrobenzoic acid in 14 alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 3-methyl-1-butanol, 1-hexanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and one cyclic ether (tetrahydrofuran), and in four alkyl alkanoates (methyl ethanoate, ethyl ethanoate, propyl ethanoate, and butyl ethanoate) at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 2-chloro-5-nitrobenzoic acid. The authors were able to assemble a total of 35 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham Model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 2-chloro-5-nitrobenzoic acid, $\log_{10} c_{1,\mathrm{W}} = -2.588$ (corrected for ionization), was determined by the authors as part of their experimental study. The McGowan volume of 2-chloro-5-nitrobenzoic acid, $V = 1.2283$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 1.250$. This left four solute descriptors (S, A, B, and L) still to be determined. The 35 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 1.400$, $A = 0.670$, $B = 0.460$, and $L = 6.513$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -9.538$ for the logarithm of the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.104 and 0.124 $\log_{10}$ units, respectively.

After the 2-chloro-5-nitrobenzoic acid solubility study was published, Abraham model correlations were developed for 2-pentanol, 3-methyl-1-butanol, methyl ethanoate, propyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 2-chloro-5-nitrobenzoic acid solubility data. Table 23 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 2-chloro-5-nitrobenzoic acid, x_1, determined by Stovall *et al.*,[13] were converted into molar

TABLE 23. Comparison between observed and calculated molar solubilities of 2-chloro-5-nitrobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\text{exp}}$	$\log_{10} c_1^{\text{calc}}$; Eq. (20)	$\log_{10} c_1^{\text{calc}}$; Eq. (21)
Ethanol	0.146	0.076	0.070
1-Propanol	−0.022	−0.055	−0.047
2-Propanol	0.045	−0.062	−0.046
1-Butanol	−0.111	−0.153	−0.140
2-Butanol	−0.134	−0.138	−0.151
2-Methyl-1-propanol	−0.204	−0.207	−0.288
2-Methyl-2-propanol	0.070	−0.099	−0.050
1-Pentanol	−0.134	−0.164	−0.158
2-Pentanol	−0.125	−0.192	−0.186
3-Methyl-1-butanol	−0.173	−0.273	−0.264
1-Hexanol	−0.198	−0.207	−0.210
1-Heptanol	−0.269	−0.237	−0.233
1-Octanol	−0.324	−0.256	−0.331
1-Decanol	−0.411	−0.360	−0.341
1,1′-Oxybisethane	−0.171	−0.269	−0.178
Tetrahydrofuran	0.461	0.589	0.563
Methyl ethanoate	−0.070	−0.065	−0.052
Ethyl ethanoate	−0.126	−0.051	−0.051
Propyl ethanoate	−0.289	−0.128	−0.146
Butyl ethanoate	−0.410	−0.207	−0.241

solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\text{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\text{solvent}}]$). The molar volume of the hypothetical subcooled liquid 2-chloro-5-nitrobenzoic acid is $V_{\text{solute}} = 130.38\ \text{cm}^3\ \text{mol}^{-1}$. Examination of the numerical entries in Table 23 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

The experimental solubility data for 2-chloro-5-nitrobenzoic acid in organic solvents are in Secs. 21.2–21.4.

21.2. 2-Chloro-5-nitrobenzoic acid solubility data in esters

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9290	0.07096

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9244	0.07561

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9401	0.05988

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.5%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9374	0.06260

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9170	0.08295

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

21.3. 2-Chloro-5-nitrobenzoic acid solubility data in ethers

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9415	0.05852

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9738	0.02621

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9837	0.01630

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7256	0.2744

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

21.4. 2-Chloro-5-nitrobenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) Ethanol; C_2H_6O; [64-17-5]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9086	0.09140

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 1-Propanol; C_3H_8O; [71-23-8]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9245	0.07550

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3]
(2) 2-Propanol; C_3H_8O; [67-63-0]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9025	0.09750

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9265	0.07350

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9131	0.08685

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9405	0.05947

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8842	0.1158

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9189	0.08109

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9165	0.08349

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9252	0.07483

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9202	0.07980

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3]
(2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9242	0.07584

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9259	0.07409

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 2-Chloro-5-nitrobenzoic acid; $C_7H_4ClNO_4$; [2516-96-3]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9274	0.07261

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

22. Solubility of 4-Chloro-3,5-dinitrobenzoic Acid in Organic Solvents

22.1. Critical evaluation of experimental solubility data

There has been only a single publication reporting the solubility of 4-chloro-3,5-dinitrobenzoic acid in organic solvents. Chantooni and Kolthoff[83] determined the solubility of 4-chloro-3,5-dinitrobenzoic acid in methanol and ethanenitrile at 298 K. It is not possible to perform a critical evaluation of the experimental data as measurements at only a single temperature, and there are no independent experimental solubility data for 4-chloro-3,5-dinitrobenzoic acid in either methanol or ethanenitrile.

The experimental solubility data for 4-chloro-3,5-dinitrobenzoic acid in organic solvents are in Secs. 22.2 and 22.3.

22.2. 4-Chloro-3,5-dinitrobenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 4-Chloro-3,5-dinitrobenzoic acid; $C_7H_3ClN_2O_6$; [118-97-8] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.55 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

22.3. 4-Chloro-3,5-dinitrobenzoic acid solubility data in miscellaneous organic solvents

Components:	Original Measurements:
(1) 4-Chloro-3,5-dinitrobenzoic acid; $C_7H_3ClN_2O_6$; [118-97-8] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.22 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from aqueous ethanol solution.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

23. Solubility of 4-Chloro-3-nitrobenzoic Acid in Organic Solvents

23.1. Critical evaluation of experimental solubility data

There have been several published studies[13,54,63,76,83] investigating the solubility behavior of 4-chloro-3-nitrobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Stovall *et al.*[13] measured the solubility of 4-chloro-3-nitrobenzoic acid in 17 alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 3-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, 2-ethyl-1-hexanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane), and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in six alkyl alkanoates (methyl ethanoate, ethyl ethanoate, propyl ethanoate, butyl ethanoate, pentyl ethanoate, and methyl butanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 4-chloro-3-nitrobenzoic acid. The authors were able to assemble a total of 37 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 4-chloro-3-nitrobenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -3.00$.[136] The McGowan volume of 4-chloro-3-nitrobenzoic acid, $V = 1.2283$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 1.250$. This left four solute descriptors (*S, A, B*, and *L*) still to be determined. The 37 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 1.470$, $A = 0.700$, $B = 0.440$, and $L = 6.685$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -10.21$ for the logarithm of the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.063 and 0.072 $\log_{10}$ units, respectively.

After the 4-chloro-3-nitrobenzoic acid solubility study was published, several additional Abraham model correlations have been developed, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 4-chloro-3-nitrobenzoic acid solubility data. Table 24 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 4-chloro-3-nitrobenzoic acid, x_1, determined by Stovall *et al.*[13] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1V_1 + (1-x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 4-chloro-3-nitrobenzoic acid is $V_{\mathrm{solute}} = 130.38\ \mathrm{cm^3\ mol^{-1}}$. Examination of the numerical entries in Table 24 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Chantooni and Kolthoff[76,83] determined the solubility of 4-chloro-3-nitrobenzoic acid in methanol, 2-propanol, 2-methyl-2-propanol, 1-hexanol, and ethanenitrile by titrating an aliquot of the saturated solutions with a standardized base titrant. The molar solubilities reported by the authors for 4-chloro-3-nitrobenzoic acid dissolved in 2-propanol, $c_1 = 0.436\ \mathrm{mol\ dm^{-3}}$, in 2-methyl-2-propanol, $c_1 = 0.511\ \mathrm{mol\ dm^{-3}}$, and in 1-hexanol, $c_1 = 0.283\ \mathrm{mol\ dm^{-3}}$, are in reasonable agreement with the values of $c_1 = 0.386\ \mathrm{mol\ dm^{-3}}$ (for 2-propanol), $c_1 = 0.367\ \mathrm{mol\ dm^{-3}}$ (for 2-methyl-2-propanol), and $c_1 = 0.265\ \mathrm{mol\ dm^{-3}}$ (for 1-hexanol) calculated from the mole fraction solubility data of Stovall *et al.*[13] The deviations between the two sets of experimental measurements are attributed in part to differences in chemical purities and experimental methodologies.

TABLE 24. Comparison between observed and calculated molar solubilities of 4-chloro-3-nitrobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Methanol	−0.152[a]	−0.288	−0.276
Ethanol	−0.290	−0.327	−0.303
1-Propanol	−0.433	−0.456	−0.421
2-Propanol	−0.413	−0.459	−0.416
1-Butanol	−0.510	−0.555	−0.511
2-Butanol	−0.499	−0.536	−0.527
2-Methyl-1-propanol	−0.728	−0.689	−0.657
2-Methyl-2-propanol	−0.435	−0.486	−0.414
1-Pentanol	−0.561	−0.580	−0.543
2-Pentanol	−0.525	−0.616	−0.569
3-Methyl-1-butanol	−0.627	−0.696	−0.640
1-Hexanol	−0.577	−0.619	−0.593
1-Heptanol	−0.609	−0.637	−0.614
1-Octanol	−0.642	−0.657	−0.711
1-Decanol	−0.733	−0.780	−0.731
1,1′-Oxybisethane	−0.632	−0.657	−0.533
Tetrahydrofuran	0.280	0.242	0.247
1,4-Dioxane	0.165	0.033	0.060
Methyl ethanoate	−0.365	−0.428	−0.371
Ethyl ethanoate	−0.450	−0.417	−0.386
Propyl ethanoate	−0.592	−0.498	−0.486
Butyl ethanoate	−0.641	−0.580	−0.585

[a] Experimental value is from Chantooni and Kolthoff.[83]

The experimental solubility data for 4-chloro-3-nitrobenzoic acid in organic solvents are in Secs. 23.2–23.7.

23.2. 4-Chloro-3-nitrobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54] C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000218

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

23.3. 4-Chloro-3-nitrobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9993	0.000678

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error, by compiler).

23.4. 4-Chloro-3-nitrobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9648	0.03520

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1]
(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9647	0.03534

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1]
(2) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9703	0.02966

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.5%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1]
(2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]

Original Measurements:
[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9697	0.03029

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9758	0.02420

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Methyl butanoate; $C_5H_{10}O_2$; [623-42-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9759	0.02410

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9637	0.03631

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

23.5. 4-Chloro-3-nitrobenzoic acid solubility data in ethers

Components:	Original Measurements:
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9754	0.02459

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9871	0.01289

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9913	0.008711

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8290	0.1710

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.802	0.198

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8661	0.1339

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.852	0.148

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

23.6. 4-Chloro-3-nitrobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.705 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Baker Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 343 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Ethanol; C_2H_6O; [54-17-5]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9665	0.03348

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Propanol; C_3H_8O; [71-23-8]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9719	0.02812

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Propanol; C_3H_8O; [67-63-0]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9696	0.03036

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Propanol; C_3H_8O; [67-63-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.436 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Baker Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K before use.
(2) Purity not given, Fisher Scientific, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9713	0.02874

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9704	0.02962

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9825	0.01747

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9649	0.03509

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.511 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Baker Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K before use.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9700	0.03001

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9671	0.03290

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9739	0.02606

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9668	0.03320

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.283 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Baker Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K before use.
(2) Yellow Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9764	0.02356

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9711	0.02890

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:

(1) 99.5%, Acros Organics, USA, was used as received.

(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9652	0.03481

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:

(1) 99.5%, Acros Organics, USA, was used as received.

(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9641	0.03589

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:

(1) 99.5%, Acros Organics, USA, was used as received.

(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9760	0.02399

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9649	0.03507

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

23.7. 4-Chloro-3-nitrobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[13]D. M. Stovall, C. Givens, S. Keown, K. R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **43**, 351 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9866	0.01343

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 292 nm.

Source and Purity of Chemicals:
(1) 99.5%, Acros Organics, USA, was used as received.
(2) 99.7%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Chloro-3-nitrobenzoic acid; $C_7H_4ClNO_4$; [96-99-1] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.133 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Baker Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K before use.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

24. Solubility of 4-Cyanobenzoic Acid in Organic Solvents

24.1. Critical evaluation of experimental solubility data

There is only a single published study regarding the solubility behavior of 4-cyanobenzoic acid in organic solvents. Wang and Zhang[97] measured the mole fraction solubilities in ethanol as a function of temperature using a static and dynamic method. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 25, along with the MRD calculated according to Eq. (24). Examination of the numerical entries in the last column of Table 25 reveals that the static experimental method yielded slightly more consistent experimental values as evidenced by the smaller MRD. In the case of the 4-cyanobenzoic acid solubility data, there is a noticeable difference between the two experimental methods. The relative difference can be fairly large at times. For example, the static method gave a mole fraction solubility of $x_1 = 0.03533$ for 4-cyanobenzoic acid dissolved in ethanol at 313.15 K, versus a value of $x_1 = 0.03879$ determined with the dynamic method. The calculated relative difference between the two reported values is just under 10%.

The experimental solubility data for 4-cyanobenzoic acid in organic solvents are in Sec. 24.2.

TABLE 25. Parameters of the Modified Apelblat equation for describing the solubility of 4-cyanobenzoic acid in ethanol[a]

Solvent	A	B	C	MRD (%)
Ethanol (dynamic method)	−2.476	−2523	2.062	3.794
Ethanol (static method)	−4.654	−2487	2.420	2.992

[a] Values of the coefficients and the mean relative deviations were taken from Wang and Zhang.[97]

24.2. 4-Cyanobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Cyanobenzoic acid; $C_8H_5NO_2$; [619-65-8] (2) Ethanol; C_2H_6O; [64-17-5]	[97] H. Wang and W. Zhang, J. Chem. Eng. Data **54**, 1942 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9786	0.02136
303.2	0.9734	0.02657
308.2	0.9669	0.03305
313.2	0.9647	0.03533
318.2	0.9560	0.04404

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.
[c] Solubility determined by the static method.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9764	0.02363
303.2	0.9748	0.02518
308.2	0.9693	0.03075
313.2	0.9612	0.03879
318.2	0.9569	0.04311

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.
[c] Solubility determined by the dynamic method.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water-jacketed glass vessel, thermometer, analytical balance, laser monitoring system.
Solubilities were determined using both a static and dynamic method. In the static method, excess solute and solvent were placed in a water-jacketed vessel allowed to equilibrate with stirring for three days at constant temperature. Samples of the saturated liquid phase were decanted into Petri dishes of known mass and weighed. The samples were then evaporated to dryness and the solubility determined from the mass of the solid residue and the mass of the sample analyzed. In the dynamic method, an excess of carboxylic acid was added to a known mass of ethanol. The resulting suspension was stirred in a water-jacketed vessel for 1 h at constant temperature. A known mass of ethanol was added to the vessel through a buret until the solute completely dissolved. The dissolution was monitored with a laser monitoring system. When the last portion of solid solute disappeared, the penetrated light intensity reached its maximum value. The mass of the added solvent was recorded. The solubility of the carboxylic acid was calculated from the known masses of solute and ethanol.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, Milwaukee, WI, USA, no purification details provided.
(2) 99.55%, Tianjin Kewei Chemical Reagent, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: Authors report that the uncertainty in the solubility values is estimated to be ±0.5%. The differences between the experimental values based on the static and dynamic solubility methods are considerably larger, and more on the order of ±5% to 10% (relative error).

25. Solubility of 3,5-Diaminobenzoic Acid in Organic Solvents

25.1. Critical evaluation of experimental solubility data

There is only a single published study regarding the solubility behavior of 3,5-diaminobenzoic acid in organic solvents. Wang and Zhang[97] measured the mole fraction solubilities in ethanol as a function of temperature using a static and dynamic method. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (*A*, *B*, and *C*) are given in Table 26, along with the MRD calculated according to Eq. (24). Examination of the numerical entries in the last column of Table 26 reveals that the static experimental method yielded more consistent experimental values as documented by the smaller MRD. In the case of the 3,5-diaminobenzoic acid solubility data, there is a noticeable difference between the two experimental methods. The relative difference can be fairly large at times. For example, the static method gave a mole fraction solubility of $x_1 = 0.003336$ for 3,5-diaminobenzoic acid in ethanol at 298.15 K, versus a value of $x_1 = 0.002112$ determined with the dynamic method. The calculated relative difference between the two reported values is more than 35%.

The experimental solubility data for 3,5-diaminobenzoic acid in organic solvents are in Sec. 25.2.

25.2. 3,5-Diaminobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3,5-Diaminobenzoic acid; $C_7H_8N_2O_2$; [535-87-5] (2) Ethanol; C_2H_6O; [64-17-5]	[97]H. Wang and W. Zhang, J. Chem. Eng. Data **54**, 1942 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

TABLE 26. Parameters of the Modified Apelblat equation for describing the solubility of 3,5-diaminobenzoic acid in ethanol[a]

Solvent	*A*	*B*	*C*	MRD (%)
Ethanol (dynamic method)	44.98	−4433	−5.516	10.43
Ethanol (static method)	−8.322	−1580	2.188	3.305

[a]Values of the coefficients and the mean relative deviations were taken from Wang and Zhang.[97]

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9967	0.003336
303.2	0.9966	0.003419
308.2	0.9960	0.003999
313.2	0.9956	0.004405
318.2	0.9948	0.005192

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.
[c]Solubility determined by the static method.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9979	0.002112
303.2	0.9963	0.003737
308.2	0.9962	0.003776
313.2	0.9960	0.003994
318.2	0.9953	0.004716

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.
[c]Solubility determined by the dynamic method.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water-jacketed glass vessel, thermometer, analytical balance, laser monitoring system.
Solubilities were determined using both a static and dynamic method. In the static method, excess solute and solvent were placed in a water-jacketed vessel allowed to equilibrate with stirring for three days at constant temperature. Samples of the saturated liquid phase were decanted into Petri dishes of known mass and weighed. The samples were then evaporated to dryness and the solubility determined from the mass of the solid residue and the mass of the sample analyzed. In the dynamic method, an excess of carboxylic acid was added to a known mass of ethanol. The resulting suspension was stirred in a water-jacketed vessel for 1 h at constant temperature. A known mass of ethanol was added to the vessel through a buret until the solute completely dissolved. The dissolution was monitored with a laser monitoring system. When the last portion of solid solute disappeared, the penetrated light intensity reached its maximum value. The mass of the added solvent was recorded. The solubility of the carboxylic acid was calculated from the known masses of solute and ethanol.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, Milwaukee, WI, USA, no purification details provided.
(2) 99.55%, Tianjin Kewei Chemical Reagent, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: Authors report that the uncertainty in the solubility values is estimated to be ±0.5%. The differences between the experimental values based on the static and dynamic solubility methods are considerably larger, and more on the order of ±10% to 30% (relative error).

26. Solubility of 2,4-Dichlorobenzoic Acid in Organic Solvents

26.1. Critical evaluation of experimental solubility data

There have been very few published solubility studies[83,97] involving 2,4-dichlorobenzoic acid in organic solvents. Chantooni and Kolthoff[83] determined the solubility of 2,4-dichlorobenzoic acid in methanol, ethanenitrile and *N*,*N*-dimethylformamide at 298.15 K. Wang and Zhang[97] measured the mole fraction solubilities in ethanol as a function of temperature using a static and dynamic method. The internal consistency of the ethanol datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (*A*, *B*, and *C*) are given in Table 27, along with the MRD calculated according to Eq. (24). Examination of the numerical entries in the last column of Table 27 reveals that the static experimental method yielded more consistent experimental values. In the case of the 2,4-dichlorobenzoic acid solubility data, there is a noticeable difference between the two experimental methods. The relative difference can be fairly large at times. For example, the static method gave a mole fraction solubility of $x_1 = 0.06087$ for 2,4-dichlorobenzoic acid in ethanol at 298.15 K, versus a value of $x_1 = 0.05012$ determined with the dynamic method. The calculated relative difference between the two reported values is more than 15%.

The experimental solubility data for 2,4-dichlorobenzoic acid in organic solvents are in Secs. 26.2 and 26.3.

26.2. 2,4-Dichlorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [50-84-0] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
$T/\mathrm{K} = 298.15$	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.34 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

TABLE 27. Parameters of the Modified Apelblat equation for describing the solubility of 2,4-dichlorobenzoic acid in ethanol[a]

Solvent	*A*	*B*	*C*	MRD (%)
Ethanol (dynamic method)	−1.902	−2652	2.183	5.661
Ethanol (static method)	3.819	−2942	1.367	0.995

[a] Values of the coefficients and the mean relative deviations were taken from Wang and Zhang.[97]

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [50-84-0] (2) Ethanol; C_2H_6O; [64-17-5]	[97]H. Wang and W. Zhang, J. Chem. Eng. Data **54**, 1942 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9419	0.05812
303.2	0.9307	0.06933
308.2	0.9183	0.08166
313.2	0.9047	0.09534
318.2	0.8821	0.1179

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.
[c] Solubility determined by the static method.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9519	0.04814
303.2	0.9322	0.06785
308.2	0.9291	0.07093
313.2	0.9193	0.08072
318.2	0.8944	0.1056

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.
[c] Solubility determined by the dynamic method.

Auxiliary Information

Method/Apparatus/Procedure:

Thermostated water-jacketed glass vessel, thermometer, analytical balance, laser monitoring system.

Solubilities were determined using both a static and dynamic method. In the static method, excess solute and solvent were placed in a water-jacketed vessel allowed to equilibrate with stirring for three days at constant temperature. Samples of the saturated liquid phase were decanted into Petri dishes of known mass and weighed. The samples were then evaporated to dryness and the solubility determined from the mass of the solid residue and the mass of the sample analyzed. In the dynamic method, an excess of carboxylic acid was added to a known mass of ethanol. The resulting suspension was stirred in a water-jacketed vessel for 1 h at constant temperature. A known mass of ethanol was added to the vessel through a buret until the solute completely dissolved. The dissolution was monitored with a laser monitoring system. When the last portion of solid solute disappeared, the penetrated light intensity reached its maximum value. The mass of the added solvent was recorded. The solubility of the carboxylic acid was calculated from the known masses of solute and ethanol.

Source and Purity of Chemicals:

(1) 98%, Sigma-Aldrich Chemical Company, Milwaukee, WI, USA, no purification details provided.

(2) 99.55%, Tianjin Kewei Chemical Reagent, China, no information given regarding any further purification.

Estimated Error:

Temperature: ±0.1 K.

x_1: Authors report that the uncertainty in the solubility values is estimated to be ±0.5%. The differences between the experimental values based on the static and dynamic solubility methods are considerably larger, and more on the order of ±5% to 15% (relative error).

26.3. 2,4-Dichlorobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 2,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [50-84-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.168 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.

(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [50-84-0] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.93 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.

(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

c_1: ±2% (relative error, estimated by compiler).

27. Solubility of 3,4-Dichlorobenzoic Acid in Organic Solvents

27.1. Critical evaluation of experimental solubility data

There have been several studies[54,63,76,83,137] that have reported the solubility of 3,4-dichlorobenzoic acid in organic solvents. Wilson *et al.*[137] determined the solubility of 3,4-dichlorobenzoic acid in 16 alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol and 1-octanol), in six alkyl alkanoates (methyl ethanoate, ethyl ethanoate, propyl ethanoate, butyl ethanoate, pentyl ethanoate and methyl butanoate), in four dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, 1,1′-oxybisbutane, and 2-methoxy-2-methylpropane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in five alkoxyalcohols (2-ethoxyethanol, 2-propoxyethanol, 2-isopropoxyethanol, 2-butoxyethanol and 3-methoxy-1-butanol). The solubilities were measured at single temperature of 298 K. The authors determined the solubilities to check the numerical values of the solute descriptors of 3,4-dichlorobenzoic acid that had been calculated previously based on limited water-to-organic solvent partition coefficient data.

An indication of the consistency of the experimental data can be gained by comparing the measured solubility data to predicted values based on the Abraham model Eqs. (20) and (21).

Numerical values of the solute descriptors for 3,4-dichlorobenzoic acid are known ($E = 0.950$, $S = 0.920$, $A = 0.670$, $B = 0.260$, $V = 1.1766$ and $L = 5.623$), so that combination of these descriptors with the coefficients listed in Tables 1 and 2 enables the prediction of $\log_{10}(c_{1,\mathrm{S}}/c_{1,\mathrm{W}})$ and $\log_{10}(c_{1,\mathrm{S}}/c_{1,\mathrm{G}})$. The molar solubility of molecular 3,4-dichlorobenzoic acid in water, $\log_{10} c_{1,\mathrm{W}} = -3.98$, is available to convert the predicted $(c_{1,\mathrm{S}}/c_{1,\mathrm{W}})$ solubility ratios to $c_{1,\mathrm{S}}$ values. For carboxylic acid solutes, $c_{1,\mathrm{W}}$ corresponds to the aqueous solubility of the molecular, nonionized form of the solute. The aqueous solubility was determined by adding two drops of hydrochloric acid to suppress ionization. Similarly, the numerical value of $\log_{10} c_{1,\mathrm{G}}$ is known ($\log_{10} c_{1,\mathrm{G}} = -8.72$) for converting predicted $(c_{1,\mathrm{S}}/c_{1,\mathrm{G}})$ solubility ratios to $c_{1,\mathrm{S}}$ values.

The predicted molar solubilities of 3,4-dichlorobenzoic acid in methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, 1-octanol, 2-propanol, 2-butanol, 2-pentanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 3-methyl-1-butanol, 1,1′-oxybisethane, 2-methoxy-2-methylpropane, tetrahydrofuran, 1,4-dioxane, methyl ethanoate, ethyl ethanoate, propyl ethanoate and butyl ethanoate are listed in the third and fourth columns of Table 28. The numerical values represent outright solubility predictions in that none of the experimental data was used in the determination of the molecular solute descriptors. For comparison purposes, the measured mole fraction solubilities of 3,4-dichlorobenzoic acid, x_1, determined by Wilson *et al.*[137] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 3,4-dichlorobenzoic acid, $V_{\mathrm{solute}} = 129.78\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$, was estimated as the molar volume of benzoic acid ($V_{\mathrm{benzoic\ acid}} = 104.38\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$) plus two times the molar volume of chlorobenzene ($V_{\mathrm{chlorobenzene}} = 102.1\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$) minus two times the molar volume of benzene ($V_{\mathrm{benzene}} = 89.40\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$). Any errors resulting from the estimation of 3,4-dichlorobenzoic acid's hypothetical subcooled liquid molar volume, V_{Solute}, or the ideal molar volume approximation will have negligible effect of the calculated c_1 values because 3,4-dichlorobenzoic acid is not overly soluble in many of the solvents considered. From a mathematical standpoint, the $x_1^{\mathrm{exp}}V_{\mathrm{Solute}}$ term contributes very little to the molar volumes of the saturated solutions. The molar solubility of 3,4-dichlorobenzoic acid, $\log_{10} c_1 = -0.569$, in methanol in Table 28 was determined by Chantooni and Kolthoff.[83]

Table 28. Comparison between observed and predicted molar solubilities of 3,4-dichlorobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Methanol	−0.569	−0.568	−0.596
Ethanol	−0.539	−0.441	−0.450
1-Propanol	−0.615	−0.527	−0.507
2-Propanol	−0.644	−0.497	−0.471
1-Butanol	−0.661	−0.598	−0.573
2-Butanol	−0.691	−0.573	−0.588
2-Methyl-1-propanol	−0.826	−0.720	−0.732
2-Methyl-2-propanol	−0.442	−0.483	−0.418
1-Pentanol	−0.699	−0.565	−0.541
2-Pentanol	−0.647	−0.550	−0.545
3-Methyl-1-butanol	−0.708	−0.628	−0.639
1-Hexanol	−0.722	−0.606	−0.601
1-Heptanol	−0.752	−0.593	−0.607
1-Octanol	−0.814	−0.664	−0.707
1,1′-Oxybisethane	−0.535	−0.609	−0.547
2-Methoxy-2-methylpropane	−0.523	−0.632	−0.805
Tetrahydrofuran	0.067	0.029	0.017
1,4-Dioxane	−0.251	−0.362	−0.350
Methyl ethanoate	−0.829	−0.752	−0.710
Ethyl ethanoate	−0.781	−0.573	−0.574
Propyl ethanoate	−0.818	−0.632	−0.652
Butyl ethanoate	−0.809	−0.692	−0.730

Examination of the numerical entries in Table 28 reveals that expressions based on the Abraham model provide a very reasonable estimation of the solubility behavior of 3,4-dichlorobenzoic acid in 1,1′-oxybisethane, 2-methoxy-2-methylpropane, tetrahydrofuran, 1,4-dioxane, and in 15 alcohol and four alkyl ethanoate solvents. Standard deviations between predicted and observed values were on the order of 0.12 and 0.13 $\log_{10}$ units for Eqs. (20) and (21), respectively. 1,1′-Oxybisbutane was excluded from the comparison because of concerns regarding possible dimerization of 3,4-dichlorobenzoic acid due to the presence of the larger alkyl chains. Solubility predictions were not made for 2-methyl-1-butanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 2,2′-oxybispropane, pentyl ethanoate, methyl butanoate, and the five alkoxyalcohols due to lack of Abraham model equation coefficients.

Hancock *et al.*[54,63] measured the solubility of 3,4-dichlorobenzoic acid in cyclohexane, benzene, tetrahydrofuran and 1,4-dioxane at 303 K. Chantooni and Kolthoff[76,83] determined the solubility of 3,4-dichlorobenzoic acid in methanol, 2-propanol, 2-methyl-2-propanol, 1-hexanol, ethanenitrile, dimethyl sulfoxide, and *N*,*N*-dimethylformamide at 298 K. The solubility data of Chantooni and Kolthoff of $\log_{10} c_1 = -0.499$ for 2-propanol, $\log_{10} c_1 = -0.438$ for 2-methyl-2-propanol, and $\log_{10} c_1 = -0.569$ for 1-hexanol are in reasonably good agreement with the experimental values of Wilson *et al.*[137] and predicted values based on Eqs. (20) and (21) which are given in Table 28. The deviations between the two sets of experimental measurements are attributed in part to differences in chemical purities and experimental methodologies.

The experimental solubility data for 3,4-dichlorobenzoic acid in organic solvents are in Secs. 27.2–27.8.

27.2. 3,4-Dichlorobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000578

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

27.3. 3,4-Dichlorobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9993	0.000734

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error, by compiler).

27.4. 3,4-Dichlorobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[b]	x_1[c]
0.9881	0.01192

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9836	0.01641

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9824	0.01761

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9794	0.02056

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9784	0.02156

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Methyl butanoate; $C_5H_{10}O_2$; [623-42-7]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9857	0.01430

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

27.5. 3,4-Dichlorobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9692	0.03077

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9874	0.01256

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9903	0.00969

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Methoxy-2-methylpropane; $C_5H_{12}O$; [1634-04-4]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9642	0.03583

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8993	0.1007

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.875	0.125

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9507	0.04931

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.943	0.057

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

27.6. 3,4-Dichlorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.27 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, synthesized by the authors by the oxidation of 3,4-dichlorobenzaldehyde with hydrogen peroxide in dilute aqueous sodium hydroxide solution. The sample was further purified by recrystallization from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Ethanol; C_2H_6O; [64-17-5]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9827	0.01732

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) Absolute, Aaper Alcohol Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1-Propanol; C_3H_8O; [71-23-8]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9815	0.01846

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Propanol; C_3H_8O; [67-63-0]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9823	0.01767

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Propanol; C_3H_8O; [67-63-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.317 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, synthesized by the authors by the oxidation of 3,4-dichlorobenzaldehyde with hydrogen peroxide in dilute aqueous sodium hydroxide solution. The sample was further purified by recrystallization from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Fisher Scientific, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9797	0.02026

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9810	0.01898

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9861	0.01389

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9655	0.03449

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.365 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, synthesized by the authors by the oxidation of 3,4-dichlorobenzaldehyde with hydrogen peroxide in dilute aqueous sodium hydroxide solution. The sample was further purified by recrystallization from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9782	0.02180

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9752	0.02477

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9817	0.01834

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9784	0.02157

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9762	0.02376

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.271 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, synthesized by the authors by the oxidation of 3,4-dichlorobenzaldehyde with hydrogen peroxide in dilute aqueous sodium hydroxide solution. The sample was further purified by recrystallization from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Yellow Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9761	0.02388

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9744	0.02555

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9749	0.02506

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9758	0.02419

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

27.7. 3,4-Dichlorobenzoic acid solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [111-80-5]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9554	0.04455

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9532	0.04677

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9517	0.04831

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9601	0.03991

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[137]A. Wilson, A. Tian, V. Chou, A. N. Quay, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **50**, 324 (2012).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9497	0.05033

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

27.8. 3,4-Dichlorobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.028 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, synthesized by the authors by the oxidation of 3,4-dichlorobenzaldehyde with hydrogen peroxide in dilute aqueous sodium hydroxide solution. The sample was further purified by recrystallization from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.14 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, synthesized by the authors by the oxidation of 3,4-dichlorobenzaldehyde with hydrogen peroxide in dilute aqueous sodium hydroxide solution. The sample was further purified by recrystallization from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was shaken with activated alumina and then distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-44-5] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.86 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, synthesized by the authors by the oxidation of 3,4-dichlorobenzaldehyde with hydrogen peroxide in dilute aqueous sodium hydroxide solution. The sample was further purified by recrystallization from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

28. Solubility of 3,5-Dichlorobenzoic Acid in Organic Solvents

28.1. Critical evaluation of experimental solubility data

Only one laboratory has reported solubility data for 3,5-dichlorobenzoic acid in organic solvents. Chantooni and Kolthoff[83,136] determined the solubility of 3,5-dichlorobenzoic acid in methanol and ethanenitrile at 298.15 K. It is not possible to perform a critical evaluation of the experimental data as measurements were performed at only a single temperature, and there are no independent experimental solubility data for 3,5-dichlorobenzoic acid in either methanol or ethanenitrile.

The experimental solubility data for 3,5-dichlorobenzoic acid in organic solvents are in Secs. 28.2 and 28.3.

28.2. 3,5-Dichlorobenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 3,5-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-36-5] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.25 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

28.3. 3,5-Dichlorobenzoic acid solubility data in miscellaneous organic solvents

Components:	Original Measurements:
(1) 3,5-Dichlorobenzoic acid; $C_7H_4Cl_2O_2$; [51-36-5] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[136]M. K. Chantooni, Jr. and I. M. Kolthoff, J. Phys. Chem. **78**, 839 (1974).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.085 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

29. Solubility of 2,4-Dihydroxybenzoic Acid in Organic Solvents

29.1. Critical evaluation of experimental solubility data

There is only a single study reporting solubility data for 2,4-dihydroxybenzoic acid in organic solvents. Ongley[56] determined the solubility of 2,4-dihydroxybenzoic acid in cyclohexane, benzene, trichloromethane and tetrachloromethane at 298.15 K. It is not possible to perform a critical evaluation of the experimental data as measurements were performed at only a single temperature, and there are no independent experimental solubility data for 2,4-dihydroxybenzoic acid in the aforementioned four solvents.

The experimental solubility data for 2,4-dihydroxybenzoic acid dissolved in organic solvents are in Secs. 29.2–29.4.

29.2. 2,4-Dihydroxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2,4-Dihydroxybenzoic acid; $C_7H_6O_4$; [89-86-1] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 5.000$, which corresponds to a solubility of $c_1 = 0.0000100$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

29.3. 2,4-Dihydroxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,4-Dihydroxybenzoic acid; $C_7H_6O_4$; [89-86-1] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 2.412$, which corresponds to a solubility of $c_1 = 0.00387$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

29.4. 2,4-Dihydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,4-Dihydroxybenzoic acid; $C_7H_6O_4$; [89-86-1] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.897$, which corresponds to a solubility of $c_1 = 0.0127$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2,4-Dihydroxybenzoic acid; $C_7H_6O_4$; [89-86-1] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 5.301$, which corresponds to a solubility of $c_1 = 0.00000500$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

30. Solubility of 2,5-Dihydroxybenzoic Acid in Organic Solvents

30.1. Critical evaluation of experimental solubility data

There are only two studies[56,125] reporting solubility data for 2,5-dihydroxybenzoic acid in organic solvents. Ongley[56] determined the solubility of 2,5-dihydroxybenzoic acid in benzene and trichloromethane at 298.15 K. Pinsuwan *et al.*[125] measured the solubility of 2,5-dihydroxybenzoic acid in 1-octanol to examine correlations between experimental octanol/water solubility ratios and measured water-to-1-octanol practical partition coefficients. It is not possible to perform a critical evaluation of the experimental data as measurements were performed at only a single temperature, and there are no independent experimental solubility data for 2,5-dihydroxybenzoic acid in either benzene, trichloromethane or 1-octanol.

The experimental solubility data for 2,5-dihydroxybenzoic acid in organic solvents are in Secs. 30.2–30.4.

30.2. 2,5-Dihydroxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,5-Dihydroxybenzoic acid; $C_7H_6O_4$; [470-79-9] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 3.403$, which corresponds to a solubility of $c_1 = 0.000395$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

30.3. 2,5-Dihydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,5-Dihydroxybenzoic acid; $C_7H_6O_4$; [470-79-9] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.900$, which corresponds to a solubility of $c_1 = 0.0126$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

30.4. 2,5-Dihydroxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2,5-Dihydroxybenzoic acid; $C_7H_6O_4$; [470-79-9] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[125]S. Pinsuwan, A. Li, and S. H. Yalkowsky, J. Chem. Eng. Data **40**, 623 (1995).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $\log_{10} c_1 = -0.13$, which corresponds to a molar solubility of $c_1 = 0.741$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, mechanical stirrer, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated at 298 ± 2 K in a sealed vial for 48–72 h. The solution was mixed using an end-over-end mechanical stirrer. After equilibrium was obtained, the saturated sample was vacuum filtered through a 5.0 μm fritted glass filter. An aliquot of the filtrate was diluted quantitatively with 2-propanol, and the absorbance of the diluted sample was recorded. The solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, St. Louis, MO, USA, used as received.
(2) Purity not given, Chemical source not given, used as received.

Estimated Error:
Temperature: ±2 K.
c_1: ±10% (relative error, estimated by compiler given the large uncertainty in temperature).

31. Solubility of 2,6-Dihydroxybenzoic Acid in Organic Solvents

31.1. Critical evaluation of experimental solubility data

There is only a single study reporting solubility data for 2,6-dihydroxybenzoic acid in organic solvents. Ongley[56] determined the solubility of 2,6-dihydroxybenzoic acid in cyclohexane, benzene, trichloromethane, and tetrachloromethane at 298.15 K. It is not possible to perform a critical evaluation of the experimental data as measurements were performed at only a single temperature, and there are no independent experimental solubility data for 2,6-dihydroxybenzoic acid in any of the four solvents listed above.

The experimental solubility data for 2,6-dihydroxybenzoic acid in organic solvents are in Secs. 31.2–31.4.

31.2. 2,6-Dihydroxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2,6-Dihydroxybenzoic acid; $C_7H_6O_4$; [303-07-1] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 3.627$, which corresponds to a solubility of $c_1 = 0.000236$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

31.3. 2,6-Dihydroxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,6-Dihydroxybenzoic acid; $C_7H_6O_4$; [303-07-1] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.896$, which corresponds to a solubility of $c_1 = 0.0127$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

31.4. 2,6-Dihydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,6-Dihydroxybenzoic acid; $C_7H_6O_4$; [303-07-1] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.539$, which corresponds to a solubility of $c_1 = 0.289 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2,6-Dihydroxybenzoic acid; $C_7H_6O_4$; [303-07-1] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 2.556$, which corresponds to a solubility of $c_1 = 0.00278 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

32. Solubility of 3,4-Dihydroxybenzoic Acid in Organic Solvents

32.1. Critical evaluation of experimental solubility data

There is only a single study reporting solubility data for 3,4-dihydroxybenzoic acid in organic solvents. Ongley[56] determined the solubility of 3,4-dihydroxybenzoic acid in trichloromethane and tetrachloromethane at 298.15 K. It is not possible to perform a critical evaluation of the experimental data as measurements were performed at only a single temperature, and there are no independent experimental solubility data for 3,4-dihydroxybenzoic acid in either trichloromethane or tetrachloromethane.

The experimental solubility data for 3,4-dihydroxybenzoic acid in organic solvents are in Sec. 32.2.

32.2. 3,4-Dihydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3,4-Dihydroxybenzoic acid; $C_7H_6O_4$; [99-50-3] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 3.311$, which corresponds to a solubility of $c_1 = 0.000489 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dihydroxybenzoic acid; $C_7H_6O_4$; [99-50-3] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 4.398$, which corresponds to a solubility of $c_1 = 0.0000400$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

33. Solubility of 2,6-Dimethoxybenzoic Acid in Organic Solvents

33.1. Critical evaluation of experimental solubility data

There is only a single study reporting solubility data for 2,6-dimethoxybenzoic acid in organic solvents. Ongley[56] determined the solubility of 2,6-dimethoxybenzoic acid in cyclohexane, benzene, and trichloromethane at 298.15 K. It is not possible to perform a critical evaluation of the experimental data as measurements were performed at only a single temperature, and there are no independent experimental solubility data for 2,6-dimethoxybenzoic acid in the aforementioned three solvents.

The experimental solubility data for 2,6-dimethoxybenzoic acid in organic solvents are in Secs. 33.2–33.4.

33.2. 2,6-Dimethoxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2,6-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [1466-76-8] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 4.000$, which corresponds to a solubility of $c_1 = 0.000100$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

33.3. 2,6-Dimethoxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,6-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [1466-76-8] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.796$, which corresponds to a solubility of $c_1 = 0.0160$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

33.4. 2,6-Dimethoxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2,6-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [1466-76-8] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.697$, which corresponds to a solubility of $c_1 = 0.201$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

34. Solubility of 3,4-Dimethoxybenzoic Acid in Organic Solvents

34.1. Critical evaluation of experimental solubility data

There have been two published studies[138,139] investigating the solubility behavior of 3,4-dimethoxybenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Bowen *et al.*[138] measured the solubility of 3,4-dimethoxybenzoic acid in 18 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in six alkyl alkanoates (methyl ethanoate, ethyl ethanoate, propyl ethanoate, butyl ethanoate, pentyl ethanoate, and methyl butanoate), in two alkanones (propanone and butanone), in four alkoxyalcohols (2-ethoxyethanol, 2-isopropoxyethanol, 2-butoxyethanol, and 3-methoxy-1-butanol), and in propylene carbonate at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 3,4-dimethoxybenzoic acid. The authors were able to assemble a total of 52 $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) equations for which experimental partition coefficient data, solubility ratios, Abraham Model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 3,4-dimethoxybenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -2.495$ (measured by the authors as part of the experimental study). The McGowan volume of 3,5-dimethoxybenzoic acid, $V = 1.3309$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.950$. This left four solute descriptors (S, A, B and L) still to be determined. The 52 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 1.646$, $A = 0.570$, $B = 0.755$, and $L = 6.746$, that best described the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -10.942$ for the gas-phase solute concentration that made the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values to within an average standard deviation of 0.084 and 0.082 $\log_{10}$ units, respectively.

Table 29 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 3,4-dimethoxybenzoic acid, x_1, determined by Bowen *et al.*[138] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 3,4-dimethoxybenzoic acid

TABLE 29. Comparison between observed and calculated molar solubilities of 3,4-dimethoxybenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\text{exp}}$	$\log_{10} c_1^{\text{calc}}$; Eq. (20)	$\log_{10} c_1^{\text{calc}}$; Eq. (21)
Methanol	−0.735	−0.721	−0.685
Ethanol	−0.916	−0.924	−0.892
1-Propanol	−1.070	−1.062	−1.061
2-Propanol	−1.097	−1.085	−1.064
1-Butanol	−1.169	−1.186	−1.173
2-Butanol	−1.154	−1.099	−1.104
2-Methyl-1-propanol	−1.315	−1.204	−1.200
2-Methyl-2-propanol	−1.001	−1.106	−1.080
1-Pentanol	−1.267	−1.269	−1.267
2-Pentanol	−1.267	−1.256	−1.230
3-Methyl-1-butanol	−1.293	−1.182	−1.258
1-Hexanol	−1.309	−1.302	−1.296
1-Heptanol	−1.362	−1.362	−1.341
1-Octanol	−1.410	−1.379	−1.443
1-Decanol	−1.501	−1.563	−1.547
1,1′-Oxybisethane	−1.525	−1.378	−1.443
Tetrahydrofuran	−0.328	−0.520	−0.546
1,4-Dioxane	−0.480	−0.608	−0.635
Propylene carbonate	−1.029	−1.006	−0.981
Methyl ethanoate	−0.973	−0.899	−0.946
Ethyl ethanoate	−1.085	−1.128	−1.101
Propyl ethanoate	−1.229	−1.205	−1.182
Butyl ethanoate	−1.303	−1.283	−1.263

is $V_{\text{solute}} = 143.8\ \text{cm}^3\ \text{mol}^{-1}$. Examination of the numerical entries in Table 29 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Li *et al.*[139] measured the solubility of 3,4-dimethoxybenzoic acid in five alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, and 2-methyl-1-propanol), two alkyl ethanoates (methyl ethanoate and ethyl ethanoates) and one alkanone (2-butanone) over the temperature range from 278 to 323 K. The internal consistency of the eight datasets was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model [Eq. (8)]. The values of the equation coefficients (A, B, and C) are given in Table 30, along with the mean relative deviation. Examination of the numerical values in the last column of Table 30 indicates that Eq. (8) provides a reasonably accurate mathematical description of how the solubility varies with temperature. The small mean relative deviations suggest that the experimental values in each solvent dataset are internally consistent.

TABLE 30. Parameters of the Modified Apelblat equation for describing the solubility of 3,4-dimethoxybenzoic acid in various organic solvents

Solvent	T/K	A	B	C	MRD (%)
Ethanol	278–323	−179.892	4830.140	27.872	0.43
1-Propanol	278–323	−120.239	1951.116	19.067	0.35
2-Propanol	278–323	−108.899	1184.711	17.518	1.10
1-Butanol	278–323	−187.012	4848.020	29.062	1.00
2-Methyl-1-propanol	278–323	−69.072	−831.534	11.649	0.77
Methyl ethanoate	278–323	−68.758	397.164	10.988	0.44
Ethyl ethanoate	278–323	−62.515	119.789	10.035	0.59
2-Butanone	279–323	−78.009	1085.742	12.277	0.20

[a] Values of the coefficients and mean relative deviations were taken from Li *et al.*[139]

The experimental solubility data for 3,4-dimethoxybenzoic acid in organic solvents are in Secs. 34.2–34.8.

34.2. 3,4-Dimethoxybenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[138] K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9915	0.00854

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[139] Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.30	0.9958	0.0042
283.01	0.9951	0.0049
288.05	0.9942	0.0058
293.15	0.9932	0.0068
298.00	0.9920	0.0080
303.13	0.9905	0.0095
308.07	0.9889	0.0111
313.15	0.9869	0.0131
318.06	0.9848	0.0152
323.37	0.9823	0.0177

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.5+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.30	0.9963	0.0037
283.01	0.9956	0.0044
288.05	0.9948	0.0052
293.15	0.9939	0.0061
298.00	0.9928	0.0072
303.13	0.9917	0.0083
308.07	0.9901	0.0099
313.15	0.9884	0.0116
318.06	0.9867	0.0133
323.37	0.9863	0.0137

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.5+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9919	0.00813

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9932	0.00682

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.5%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9934	0.00660

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.7%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9935	0.00654

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Methyl butanoate; $C_5H_{10}O_2$; [623-42-7]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9932	0.00678

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

34.3. 3,4-Dimethoxybenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9969	0.00313

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9986	0.00143

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9989	0.00112

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9606	0.03937

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9710	0.02897

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

34.4. 3,4-Dimethoxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Methanol; CH_4O; [67-56-1]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9924	0.00764

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, was used as received.

(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Ethanol; C_2H_6O; [64-17-5]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9928	0.00720

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:

(1) 99+%, Acros Organics, USA, was used as received.

(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Ethanol; C_2H_6O; [64-17-5]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.9965	0.0035
282.93	0.9958	0.0042
288.21	0.9949	0.0051
293.08	0.9938	0.0062
298.00	0.9926	0.0074
303.33	0.9907	0.0093
307.90	0.9890	0.0110
313.30	0.9864	0.0136
317.15	0.9839	0.0161
323.30	0.9798	0.0202

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.

Experimental solubilities were determined by a synthetic method. Pre-weighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.7+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Propanol; C_3H_8O; [71-23-8]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9936	0.00643

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Propanol; C_3H_8O; [71-23-8]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.37	0.9973	0.0027
283.05	0.9967	0.0033
288.39	0.9958	0.0042
293.30	0.9949	0.0051
299.00	0.9934	0.0066
303.17	0.9921	0.0079
308.27	0.9907	0.0097
313.13	0.9882	0.0118
318.15	0.9854	0.0146
323.28	0.9823	0.0177

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.8+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Propanol; C_3H_8O; [67-63-0]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9938	0.00618

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Propanol; C_3H_8O; [67-63-0]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.37	0.9976	0.0024
283.05	0.9970	0.0030
288.39	0.9961	0.0039
294.07	0.9949	0.0051
299.00	0.9937	0.0063
303.17	0.9926	0.0074
308.27	0.9905	0.0095
313.13	0.9882	0.0118
318.15	0.9850	0.0150
323.20	0.9817	0.0183

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Preweighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.7+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9937	0.00625

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
277.90	0.9976	0.0024
283.25	0.9970	0.0030
288.15	0.9963	0.0037
293.04	0.9954	0.0046
298.15	0.9943	0.0057
302.94	0.9930	0.0070
308.10	0.9912	0.0088
313.15	0.9891	0.0109
318.01	0.9865	0.0135
323.33	0.9830	0.0170

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Pre-weighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.5+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[138] K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9935	0.00651

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[138] K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9955	0.00450

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
277.90	0.9985	0.0015
283.25	0.9980	0.0020
288.15	0.9974	0.0026
293.04	0.9968	0.0032
298.15	0.9959	0.0041
302.94	0.9948	0.0052
308.10	0.9934	0.0066
313.15	0.9917	0.0083
318.01	0.9895	0.0105
323.33	0.9868	0.0132

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Pre-weighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.5+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

Components:	Original Measurements:
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9905	0.00945

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	Original Measurements:
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9938	0.00615

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9941	0.00593

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9944	0.00560

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9946	0.00541

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9938	0.00615

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9942	0.00573

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9935	0.00646

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9938	0.00617

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9938	0.00616

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9942	0.00577

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

34.5. 3,4-Dimethoxybenzoic acid solubility in alkoxyalcohols

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9696	0.03037

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9766	0.02335

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9851	0.01485

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9745	0.02547

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

34.6. 3,4-Dimethoxybenzoic acid solubility data in alkanones

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Propanone; C_3H_6O; [67-64-1]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9882	0.01177

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Butanone; C_4H_8O; [78-93-3]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9879	0.01206

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) 2-Butanone; C_4H_8O; [78-93-3]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.95	0.9932	0.0068
283.15	0.9923	0.0077
287.95	0.9911	0.0089
293.32	0.9896	0.0104
298.13	0.9880	0.0120
303.15	0.9860	0.0140
308.37	0.9838	0.0162
313.05	0.9816	0.0184
318.15	0.9788	0.0212
323.49	0.9754	0.0246

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a synthetic method. Pre-weighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.7%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error).

34.7. 3,4-Dimethoxybenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[138]K. R. Bowen, T. W. Stephens, H. Lu, K. Satish, D. Shan, W. E. Acree, Jr., and M. H. Abraham, Eur. Chem. Bull. **2**, 577 (2013).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9920	0.00799

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 286 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

34.8. 3,4-Dimethoxybenzoic acid solubility data in binary organic solvent mixtures

Components:	**Original Measurements:**
(1) 3,4-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [93-07-2] (2) Ethanol; C_2H_6O; [64-17-5] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[139]Q. Li, F. Lu, Y. Tian, S. Feng, Y. Shen, and B. Wang, J. Chem. Eng. Data **58**, 1020 (2013).
Variables:	**Prepared by:**
Temperature; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	$m_2^{(s)}$[a]	x_1[b]
277.90	0.0000	0.0024
283.25	0.0000	0.0030
288.15	0.0000	0.0037
293.04	0.0000	0.0046
298.15	0.0000	0.0057
302.94	0.0000	0.0070
308.10	0.0000	0.0088
313.15	0.0000	0.0109
318.01	0.0000	0.0135
323.33	0.0000	0.0170
278.75	0.1000	0.0028
283.26	0.1000	0.0036
288.15	0.1000	0.0045
293.18	0.1000	0.0054
298.41	0.1000	0.0067
303.15	0.1000	0.0083
308.01	0.1000	0.0102
313.15	0.1000	0.0125
317.94	0.1000	0.0152
323.12	0.1000	0.0189
278.65	0.2000	0.0030
283.15	0.2000	0.0037
288.21	0.2000	0.0045
293.18	0.2000	0.0055
298.41	0.2000	0.0069
303.35	0.2000	0.0085
308.01	0.2000	0.0103
313.15	0.2000	0.0126
317.94	0.2000	0.0152
323.10	0.2000	0.0186
277.94	0.3000	0.0029
283.05	0.3000	0.0036
288.38	0.3000	0.0045
293.45	0.3000	0.0055
298.25	0.3000	0.0067
303.55	0.3000	0.0083
308.13	0.3000	0.0101
313.15	0.3000	0.0123
318.29	0.3000	0.0150
323.06	0.3000	0.0180
279.20	0.4000	0.0029
283.45	0.4000	0.0034
288.03	0.4000	0.0043
292.91	0.4000	0.0052
298.02	0.4000	0.0064
303.66	0.4000	0.0080
307.94	0.4000	0.0095
313.10	0.4000	0.0118
318.15	0.4000	0.0143
323.05	0.4000	0.0173
279.20	0.5000	0.0034
283.45	0.5000	0.0040
288.03	0.5000	0.0048
292.91	0.5000	0.0058
298.02	0.5000	0.0071
303.66	0.5000	0.0090
307.94	0.5000	0.0106
313.10	0.5000	0.0129
318.15	0.5000	0.0156
323.05	0.5000	0.0188
278.04	0.6000	0.0032
283.16	0.6000	0.0040
288.15	0.6000	0.0049
293.14	0.6000	0.0060
298.08	0.6000	0.0073
303.13	0.6000	0.0089
307.94	0.6000	0.0108
313.05	0.6000	0.0130
318.19	0.6000	0.0160
323.33	0.6000	0.0195
278.04	0.7000	0.0034
283.16	0.7000	0.0040
288.15	0.7000	0.0050
293.14	0.7000	0.0061
298.08	0.7000	0.0074
303.13	0.7000	0.0090
307.94	0.7000	0.0109
313.05	0.7000	0.0132
318.19	0.7000	0.0161
323.33	0.7000	0.0194
278.50	0.8000	0.0034
283.15	0.8000	0.0041
288.15	0.8000	0.0050
293.16	0.8000	0.0061
298.29	0.8000	0.0077
303.22	0.8000	0.0093
308.31	0.8000	0.0115
312.99	0.8000	0.0137
318.25	0.8000	0.0168
323.42	0.8000	0.0207
278.37	0.9000	0.0035
283.05	0.9000	0.0043
288.39	0.9000	0.0051
293.16	0.9000	0.0062
298.29	0.9000	0.0077
303.22	0.9000	0.0091
308.31	0.9000	0.0112
312.99	0.9000	0.0133
318.25	0.9000	0.0162
323.42	0.9000	0.0196
278.15	1.0000	0.0035
282.93	1.0000	0.0042
288.21	1.0000	0.0051
293.08	1.0000	0.0062
298.00	1.0000	0.0074
303.33	1.0000	0.0093
307.90	1.0000	0.0110
313.30	1.0000	0.0136
317.15	1.0000	0.0161
323.30	1.0000	0.0202

[a] $m_2^{(s)}$: mass fraction of component 2 in the initial binary solvent mixture.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Water-jacketed equilibrium glass vessel, thermostated circulating water bath, magnetic stirrer, analytical balance, laser monitoring system.

Experimental solubilities were determined by a synthetic method. Pre-weighed amounts of solute and solvent and were placed in a water-jacketed equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and small amounts of solute were incrementally added until no further solid dissolved. The dissolution of the solid was determined using laser monitoring. The total amount of solute dissolved was recorded. Experimental measurement was repeated three times.

Source and Purity of Chemicals:
(1) 99+%, Alfa Aesar China Co., Ltd., Tianjin, China, no purification details were provided.
(2) 99.7+%, Beijing Chemical Works, Beijing, China, no purification details were provided.
(3) 99.5+%, Beijing Chemical Works, Beijing, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
$m_2^{(s)}$: 0.0001
x_1: ±4% (relative error).

35. Solubility of 3,5-Dimethoxybenzoic Acid in Organic Solvents

35.1. Critical evaluation of experimental solubility data

There is only a single published study regarding the solubility behavior of 3,5-dimethoxybenzoic acid in organic solvents. Wang and Zhang[97] measured the mole fraction solubilities in ethanol as a function of temperature using a static and dynamic method. The internal consistency of the two datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 31, along with the MRD calculated according to Eq. (24). Examination of the numerical entries in the last column of Table 31 reveals that the static experimental method yielded slightly more consistent experimental values as evidenced by the smaller MRD. In the case of the 3,5-dimethoxybenzoic acid solubility data, there is a slight difference between the two experimental methods. The relative difference can be greater than the reproducibility at times. For example, the static method gave a mole fraction solubility of $x_1 = 0.007464$ for 3,5-dimethoxybenzoic acid in ethanol at 308.15 K, versus a value of $x_1 = 0.007934$ determined with the dynamic method. The calculated relative difference between the two reported values is about 6%. The authors estimated the reproducibility of the measurements at 0.5%.

The experimental solubility data for 3,5-dimethoxybenzoic acid in ethanol are in Sec. 33.2.

TABLE 31. Parameters of the Modified Apelblat equation for describing the solubility of 3,5-dimethoxybenzoic acid in ethanol[a]

Solvent	A	B	C	MRD (%)
Ethanol (dynamic method)	−0.1742	−3316	1.865	2.160
Ethanol (static method)	40.45	−5379	−4.060	0.947

[a] Values of the coefficients and the mean relative deviations were taken from Wang and Zhang.[97]

35.2. 3,5-Dimethoxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3,5-Dimethoxybenzoic acid; $C_9H_{10}O_4$; [1132-21-4] (2) Ethanol; C_2H_6O; [64-17-5]	[97] H. Wang and W. Zhang, J. Chem. Eng. Data **54**, 1942 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9951	0.004933
303.2	0.9939	0.006075
308.2	0.9925	0.007464
313.2	0.9907	0.009341
318.2	0.9884	0.01159

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.
[c] Solubility determined by the static method.

Experimental Values

T/K	x_2[a]	x_1[b,c]
298.2	0.9949	0.005137
303.2	0.9939	0.006056
308.2	0.9921	0.007934
313.2	0.9902	0.009776
318.2	0.9886	0.01143

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.
[c] Solubility determined by the dynamic method.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water-jacketed glass vessel, thermometer, analytical balance, laser monitoring system.
Solubilities were determined using both a static and dynamic method. In the static method, excess solute and solvent were placed in a water-jacketed vessel allowed to equilibrate with stirring for three days at constant temperature. Samples of the saturated liquid phase were decanted into Petri dishes of known mass and weighed. The samples were then evaporated to dryness and the solubility determined from the mass of the solid residue and the mass of the sample analyzed. In the dynamic method, an excess of carboxylic acid was added to a known mass of ethanol. The resulting suspension was stirred in a water-jacketed vessel for 1 h at constant temperature. A known mass of ethanol was added to the vessel through a buret until the solute completely dissolved. The dissolution was monitored with a laser monitoring system. When the last portion of solid solute disappeared, the penetrated light intensity reached its maximum value. The mass of the added solvent was recorded. The solubility of the carboxylic acid was calculated from the known masses of solute and ethanol.

Source and Purity of Chemicals:
(1) 98%, Sigma-Aldrich Chemical Company, Milwaukee, WI, USA, no purification details provided.
(2) 99.55%, Tianjin Kewei Chemical Reagent, China, no information given regarding any further purification.

Estimated Error:
Temperature: ±0.1 K.
x_1: Authors report that the uncertainty in the solubility values is estimated to be ±0.5%. The differences between the experimental values based on the static and dynamic solubility methods are considerably larger, and more on the order of ±3% to 8% (relative error).

36. Solubility of 3-(Dimethylamino)benzoic Acid in Organic Solvents

36.1. Critical evaluation of experimental solubility data

There has been only a single study reporting the solubility of 3-(dimethylamino)benzoic acid in organic solvents. Hancock *et al.*[54] determined the solubility of 3-(dimethylamino)benzoic acid in cyclohexane and benzene at 303 K based on a gravimetric method. It is not possible to perform a critical evaluation of the experimental data as measurements were performed at only a single temperature, and there are no independent experimental solubility data for 3-(dimethylamino)benzoic acid in either cyclohexane or benzene.

The experimental solubility data for 3-(dimethylamino) benzoic acid in organic solvents are in Secs. 36.2 and 36.3.

36.2. 3-(Dimethylamino)benzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 3-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [99-64-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9996	0.000406

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

36.3. 3-(Dimethylamino)benzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [99-64-9] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9894	0.0106

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

37. Solubility of 4-(Dimethylamino)benzoic Acid in Organic Solvents

37.1. Critical evaluation of experimental solubility data

There have been two studies[54,83] reporting the solubility of 4-(dimethylamino)benzoic acid in organic solvents. Hancock *et al.*[54] determined the solubility of 4-(dimethylamino)benzoic acid in cyclohexane and benzene at 303 K based on a gravimetric method. Chantooni and Kolthoff[83] measured the solubility of 4-(dimethylamino)benzoic acid in methanol, ethanenitrile, dimethyl sulfoxide, and *N*,*N*-dimethylformamide at 298 K. It is not possible to perform a critical evaluation of the experimental data as each research group performed measurements at only a single temperature, and there are no independent experimental solubility data for 4-(dimethylamino)benzoic acid in these six organic solvents.

The experimental solubility data for 4-(dimethylamino)benzoic acid in organic solvents are in Secs. 37.2–37.5.

37.2. 4-(Dimethylamino)benzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [619-84-1] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9996	0.000406

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

37.3. 4-(Dimethylamino)benzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [619-84-1] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9994	0.000637

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

37.4. 4-(Dimethylamino)benzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [619-84-1] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.086 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from aqueous ethanol solution.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

37.5. 4-(Dimethylamino)benzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [619-84-1] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.023 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from aqueous ethanol solution.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [619-84-1] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.95 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from aqueous ethanol solution.
(2) Purity not given, Chemical source not given, was shaken with activated alumina and then distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-(Dimethylamino)benzoic acid; $C_9H_{11}NO_2$; [619-84-1] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.10 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from aqueous ethanol solution.
(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

38. Solubility of 3,4-Dimethylbenzoic Acid in Organic Solvents

38.1. Critical evaluation of experimental solubility data

There have been two studies[76,83] reporting the solubility of 3,4-dimethylbenzoic acid in organic solvents. Chantooni and Kolthoff[83] measured the solubility of 3,4-dimethylbenzoic acid in methanol, ethanenitrile, dimethyl sulfoxide, and *N*, *N*-dimethylformamide at 298 K. In a followup study, the authors[76] determined the solubility in three additional alcohol solvents (2-propanol, 2-methyl-2-propanol, and 1-hexanol). It is not possible to perform a critical evaluation of the experimental data as measurements were made at only a single temperature, and there are no independent experimental solubility data for 3,4-dimethylbenzoic acid in these seven organic solvents.

The experimental solubility data for 3,4-dimethylbenzoic acid in organic solvents are in Secs. 38.2 and 38.3.

38.2. 3,4-Dimethylbenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3,4-Dimethylbenzoic acid; $C_9H_{10}O_2$; [619-04-5] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.595 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, K and K Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dimethylbenzoic acid; $C_9H_{10}O_2$; [619-04-5] (2) 2-Propanol; C_3H_8O; [67-63-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.513 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, K and K Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Fisher Scientific, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dimethylbenzoic acid; $C_9H_{10}O_2$; [619-04-5] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.616 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) Purity not given, K and K Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dimethylbenzoic acid; $C_9H_{10}O_2$; [619-04-5] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.408 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) Purity not given, K and K Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Yellow Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

38.3. 3,4-Dimethylbenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3,4-Dimethylbenzoic acid; $C_9H_{10}O_2$; [619-04-5] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.091 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) Purity not given, K and K Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dimethylbenzoic acid; $C_9H_{10}O_2$; [619-04-5] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 3.07 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, K and K Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was shaken with activated alumina and then distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,4-Dimethylbenzoic acid; $C_9H_{10}O_2$; [619-04-5] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.19 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, K and K Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

39. Solubility of 2,4-Dinitrobenzoic Acid in Organic Solvents

39.1. Critical evaluation of experimental solubility data

There has been one study reporting the solubility of 2,4-dinitrobenzoic acid in organic solvents. Chantooni and Kolthoff[83] determined the solubility of 2,4-dinitrobenzoic acid in methanol and ethanenitrile at 298 K. It is not possible to perform a critical evaluation of the experimental data as the authors performed measurements at only a single temperature, and there are no independent experimental solubility data for 2,4-dinitrobenzoic acid in either cyclohexane or benzene.

The experimental solubility data for 2,4-dinitrobenzoic acid in organic solvents are in Secs. 39.2 and 39.3.

39.2. 2,4-Dinitrobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2,4-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [610-30-0] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 3.23 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

39.3. 2,4-Dinitrobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 2,4-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [610-30-0] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.02 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)] the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* 333 K.

(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

c_1: ±2% (relative error, estimated by compiler).

40. Solubility of 3,5-Dinitrobenzoic Acid in Organic Solvents

40.1. Critical evaluation of experimental solubility data

There have been several published studies[54,63,76,83,140] investigating the solubility behavior of 3,5-dinitrobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Hoover *et al.*[140] measured the solubility of 3,5-dinitrobenzoic acid in 13 alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 1-pentanol, 2-pentanol, 3-methyl-1-butanol, 1-hexanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in three alkyl alkanoates (ethyl ethanoate, butyl ethanoate, and pentyl ethanoate) at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 3,5-dinitrobenzoic acid. The authors were able to assemble a total of 38 $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) equations for which experimental partition coefficient data, solubility ratios, Abraham Model equation coefficients, and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 3,5-dinitrobenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -2.417$.[141,142] The McGowan volume of 3,5-dinitrobenzoic acid, $V = 1.2801$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 1.250$. This left four solute descriptors (S, A, B, and L) still to be determined. The 38 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 1.630$, $A = 0.700$, $B = 0.590$, and $L = 6.9837$, that best described the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -10.717$ for the gas-phase solute concentration that made the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values to within an average standard deviation of 0.091 and 0.114 $\log_{10}$ units, respectively.

After the 3,5-dinitrobenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 3,5-dinitrobenzoic acid solubility data. Table 32 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 3,5-dinitrobenzoic acid, x_1, determined by Hoover *et al.*[140] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the

TABLE 32. Comparison between observed and calculated molar solubilities of 3,5-dinitrobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Ethanol	−0.128	−0.249	−0.239
1-Propanol	−0.326	−0.396	−0.385
2-Propanol	−0.366	−0.409	−0.387
1-Butanol	−0.469	−0.518	−0.498
2-Butanol	−0.496	−0.478	−0.485
2-Methyl-1-propanol	−0.655	−0.615	−0.622
1-Pentanol	−0.540	−0.562	−0.552
2-Pentanol	−0.523	−0.590	−0.564
3-Methyl-1-butanol	−0.574	−0.660	−0.627
1-Hexanol	−0.621	−0.605	−0.600
1-Heptanol	−0.653	−0.651	−0.633
1-Octanol	−0.683	−0.657	−0.735
1-Decanol	−0.746	−0.809	−0.786
1,1′-Oxybisethane	−0.555	−0.723	−0.608
Tetrahydrofuran	0.209	0.254	0.236
1,4-Dioxane	−0.005	0.102	0.104
Ethyl ethanoate	−0.311	−0.426	−0.409
Butyl ethanoate	−0.544	−0.601	−0.613

saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 3,5-dinitrobenzoic acid is $V_{\mathrm{solute}} = 131.0\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$. Examination of the numerical entries in Table 32 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Hancock *et al.*[54,63] measured the solubility of 3,5-dinitrobenzoic acid in cyclohexane, benzene, tetrahydrofuran and 1,4-dioxane at 303.15 K, which is at a slightly higher temperature than solubility data of Hoover *et al.*[140] A direct comparison is not possible since the two sets of measurements were performed a different temperatures.

The experimental solubility data for 3,5-dinitrobenzoic acid in organic solvents are in Secs. 40.2–40.7.

40.2. 3,5-Dinitrobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.00000698

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

40.3. 3,5-Dinitrobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9995	0.000454

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error, by compiler).

40.4. 3,5-Dinitrobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9511	0.04892

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9621	0.03787

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9691	0.03088

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9338	0.06616

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer
Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

40.5. 3,5-Dinitrobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9706	0.02938

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9909	0.009087

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9942	0.005787

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8569	0.1431

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.827	0.173

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9112	0.08878

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.900	0.100

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

40.6. 3,5-Dinitrobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.23 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous ethanol solution and dried *in vacuo* over barium oxide at 343 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Ethanol; C_2H_6O; [64-17-7]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9538	0.04620

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Propanol; C_3H_8O; [71-23-8]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9636	0.03637

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2-Propanol; C_3H_8O; [67-63-0]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9661	0.03390

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2-Propanol; C_3H_8O; [67-63-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.451 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous ethanol solution and dried *in vacuo* over barium oxide at 343 K.
(2) Purity not given, Fisher Scientific Chemical Company, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9683	0.03169

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9702	0.02984

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9783	0.02169

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.625 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous ethanol solution and dried *in vacuo* over barium oxide at 343 K.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9685	0.03153

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2-Pentanol; $C_5H_{10}O$; [6032-29-7]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9669	0.03308

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 3-Methyl-1-butanol; $C_5H_{10}O$; [123-51-3]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9705	0.02948

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9700	0.02997

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.357 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous ethanol solution and dried *in vacuo* over barium oxide at 343 K.
(2) Yellow Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9685	0.03147

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9673	0.03267

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[140]K. R. Hoover, R. Coaxum, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 457 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9660	0.03402

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 267 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.0212 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous ethanol solution and dried *in vacuo* over barium oxide at 343 K.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

c_1: ±2% (relative error, estimated by compiler).

40.7. 3,5-Dinitrobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3,5-Dinitrobenzoic acid; $C_7H_4N_2O_6$; [99-34-3] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.23 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous ethanol solution and dried *in vacuo* over barium oxide at 343 K.

(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

c_1: ±2% (relative error, estimated by compiler).

41. Solubility of 3,5-Dinitro-2-methylbenzoic Acid in Organic Solvents

41.1. Critical evaluation of experimental solubility data

There have been two published studies[18,143] investigating the solubility behavior of 3,5-dinitro-2-methylbenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Saifullah *et al.*[18] measured the solubility of 3,5-dinitro-2-methylbenzoic acid in tetrahydrofuran and 1,4-dioxane at 298 K. Ye *et al.*[143] measured the solubility of 3,5-dinitro-2-methylbenzoic acid in 14 alcohols (1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 3-methyl-1-butanol, 1-hexanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, and 1-decanol) and in five alkyl alkanoates (methyl ethanoate, ethyl ethanoate, propyl ethanoate, butyl ethanoate, and pentyl ethanoate) at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of

TABLE 33. Comparison between observed and calculated molar solubilities of 3,5-dinitro-2-methylbenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
1-Propanol	−0.661	−0.711	−0.690
2-Propanol	−0.712	−0.726	−0.697
1-Butanol	−0.786	−0.837	−0.800
2-Butanol	−0.784	−0.769	−0.787
2-Methyl-1-propanol	−1.054	−0.981	−0.955
2-Methyl-2-propanol	−0.820	−0.741	−0.716
1-Pentanol	−0.823	−0.966	−0.941
2-Pentanol	−0.864	−1.003	−0.942
3-Methyl-1-butanol	−0.962	−1.065	−0.955
1-Hexanol	−0.969	−0.983	−0.967
1-Heptanol	−0.925	−0.984	−1.000
1-Octanol	−1.103	−0.984	−1.095
1-Decanol	−1.336	−1.243	−1.223
Methyl ethanoate	−0.345	−0.349	−0.288
Ethyl ethanoate	−0.498	−0.550	−0.512
Butyl ethanoate	−0.703	−0.747	−0.703

3,5-dinitro-2-methylbenzoic acid. The authors were able to assemble a total of 36 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients, and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 3,5-dinitro-2-methylbenzoic acid, $\log_{10} c_{1,\mathrm{W}} = -2.60$, was determined by the authors as part of the experimental measurements. The McGowan volume of 3,5-dinitro-2-methylbenzoic acid, $V = 1.4210$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 1.310$. This left four solute descriptors (S, A, B, and L) still to be determined. The 36 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 2.120$, $A = 0.750$, $B = 0.650$, and $L = 8.040$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -12.556$ for the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.081 and 0.064 $\log_{10}$ units, respectively.

Table 33 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 3,5-dinitro-2-methylbenzoic acid, x_1, determined by Ye *et al.*[143] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 3,5-dinitro-2-methylbenzoic acid is $V_{\mathrm{solute}} = 148.4\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$. Examination of the numerical entries in Table 33 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

The experimental solubility data for 3,5-dinitro-2-methylbenzoic acid in organic solvents are in Secs. 41.2–41.4.

41.2. 3,5-Dinitro-2-methylbenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9629	0.0371

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:

(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9683	0.0317

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) Propyl ethanoate; $C_5H_{10}O_2$; [109-60-4]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9707	0.0293

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9737	0.0263

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9748	0.0252

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

41.3. 3,5-Dinitro-2-methylbenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[18]M. Saifullah, S. Ye, L. M. Grubbs, N. E. De La Rosa, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **40**, 2082 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8140	0.1860

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[18]M. Saifullah, S. Ye, L. M. Grubbs, N. E. De La Rosa, W. E. Acree, Jr., and M. H. Abraham, J. Solution Chem. **40**, 2082 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8196	0.1804

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

41.4. 3,5-Dinitro-2-methylbenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1-Propanol; C_3H_8O; [71-23-8]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9834	0.0166

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 2-Propanol; C_3H_8O; [67-63-0]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9849	0.0151

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9848	0.0152

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9847	0.0153

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9918	0.00822

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9856	0.0144

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9836	0.0164

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9850	0.0150

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9880	0.0120

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9865	0.0135

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 4-Methyl-2-butanol; $C_6H_{14}O$; [108-11-2]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9861	0.0139

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9832	0.0168

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9875	0.0125

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3,5-Dinitro-2-methylbenzoic acid; $C_8H_6N_2O_6$; [28169-46-2] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[143]S. Ye, M. Saifullah, L. M. Grubbs, M. C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **49**, 821 (2011).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9917	0.00833

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

42. Solubility of 2-Fluorobenzoic Acid in Organic Solvents

42.1. Critical evaluation of experimental solubility data

There has been only a single publication reporting the solubility of 2-fluorobenzoic acid in organic solvents. Thuaire[72] determined the solubility of 2-fluorobenzoic acid in ethanol at 298 K as part of study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. It is not possible to perform a critical evaluation of the experimental data as measurements were made at only a single temperature, and there are no independent experimental 2-fluorobenzoic acid solubility data in ethanol.

The experimental solubility data for 2-fluorobenzoic acid in ethanol is given in Sec. 42.2.

42.2. 2-Fluorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2-Fluorobenzoic acid; $C_7H_5FO_2$; [445-29-4] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.994 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1212$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

43. Solubility of 3-Fluorobenzoic Acid in Organic Solvents

43.1. Critical evaluation of experimental solubility data

There has been only a single publication reporting the solubility of 3-fluorobenzoic acid in organic solvents. Thuaire[72] determined the solubility of 3-fluorobenzoic acid in ethanol at 298 K as part of study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. It is not possible to perform a critical evaluation of the experimental data as measurements were made at only a single temperature, and there are no independent experimental 3-fluorobenzoic acid solubility data in ethanol.

The experimental solubility data for 3-fluorobenzoic acid in ethanol is given in Sec. 43.2.

43.2. 3-Fluorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Fluorobenzoic acid; $C_7H_5FO_2$; [455-38-9] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 4.746 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1794$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

44. Solubility of 4-Fluorobenzoic Acid in Organic Solvents

44.1. Critical evaluation of experimental solubility data

There have been only two publications[63,72] reporting the solubility of 4-fluorobenzoic acid in organic solvents. Hancock *et al.*[63] determined the solubility of 4-fluorobenzoic acid in tetrahydrofuran and 1,4-dioxane at 303 K based on a gravimetric method. Thuaire[72] determined the solubility in ethanol at 298 K as part of study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. It is not possible to perform a critical evaluation of the experimental data as measurements were made at only a single temperature, and there are no independent experimental 4-fluorobenzoic acid solubility data for these two organic solvents.

The experimental solubility data for 4-fluorobenzoic acid in organic solvents are given in Secs. 44.2 and 44.3.

44.2. 4-Fluorobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 4-Fluorobenzoic acid; $C_7H_5FO_2$; [456-22-4] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.811	0.189

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Fluorobenzoic acid; $C_7H_5FO_2$; [456-22-4] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.872	0.128

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

44.3. 4-Fluorobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Fluorobenzoic acid; $C_7H_5FO_2$; [456-22-4] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.438 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.06213$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

45. Solubility of 4-Formylbenzoic Acid in Organic Solvents

45.1. Critical evaluation of experimental solubility data

There have been three publications[82,84,144] reporting solubility data for 4-formylbenzoic acid. Sun *et al.*[144] measured the solubility of 4-formylbenzoic acid in ethanoic acid at 14 temperatures covering the range of 303–473 K. The internal consistency of the dataset was assessed by curve-fitting the measured mole fraction solubilities according to the Modified

Apelblat model to yield the following correlation:

$$\ln x_1 = -42.006 + \frac{114.588}{T} + 6.266 \ln T. \qquad (47)$$

Equation (47) provides a reasonably accurate mathematical description for how the solubility varies with temperature. The mean relative deviation between the observed and calculated values is 6.9%.

Dian-Qing *et al.*[82] determined the solubility of 4-formylbenzoic acid in *N*,*N*-dimethylformamide as a function of temperature using a dynamic method with laser monitoring to observe when dissolution was complete. The calculated curve-fit parameters from the Buchowski λh-model [Eq. (9)] of $\lambda = 1.398 \times 10^{-7}$ and $h = 2879.94$ described the observed solubility data from 314 to 370 K to within a mean relative deviation of 2.4%.

Li *et al.*[84] determined the solubility of 4-formylbenzoic acid dissolved in *N*-methyl-2-pyrrolidone from 296 to 341 K using a synthetic method with laser monitoring to determine when the last amount of solid solute dissolved. The authors employed a polynomial expression in temperature,

$$x = -2.4515 + 0.02776\,T - 1.10430 \times 10^{-4}\,T + 1.54936 \times 10^{-7}\,T^2, \qquad (48)$$

to represent the measured mole fraction solubility data. The root-mean-square deviation between the observed x_1 data and calculated values from Eq. (48) was on the order of 0.0005 mole fraction.

The experimental solubility data for 4-formylbenzoic acid in organic solvents are given in Sec. 45.2.

45.2. 4-Formylbenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Formylbenzoic acid; $C_8H_6O_3$; [619-66-9] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[144]W. Sun, W. Qu, and L. Zhao, J. Chem. Eng. Data **55**, 4476 (2010).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b,c]
303.2	0.9975	0.0025
323.2	0.9958	0.0042
333.2	0.9949	0.0051
343.2	0.9937	0.0063
353.2	0.9924	0.0076
363.2	0.9905	0.0095
373.2	0.9869	0.0131
403.2	0.9838	0.0162
423.2	0.9794	0.0206
433.2	0.9766	0.0234
443.2	0.9747	0.0253
453.3	0.9691	0.0309
463.3	0.9640	0.0360
473.2	0.9555	0.0445

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute, calculated by the compiler.

[c] Solubilities were given in units of grams of solute per 100 g of solvent.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed vessel made from titanium, and a high-performance liquid chromatograph equipped with an ion-exchange column.

Experimental solubilities were determined by a static method. Excess solute and solvent were placed in a jacketed vessel constructed of titanium. The solution was allowed to equilibrate several hours at constant temperature. An aliquot of the clear saturated solution was filtered and transferred to a tared volumetric flask. The concentration of the dissolved solute was determined by high-performance liquid chromatography using an ion-exchange column.

Source and Purity of Chemicals:

(1) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.

(2) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±3% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Formylbenzoic acid; $C_8H_6O_3$; [619-66-9] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[82]L. Dian-Qing, L. Jiang-Chu, L. Da-Zhuang, and W. Fu-An, Fluid Phase Equilib. **200**, 69 (2002).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
313.45	0.7761	0.2239
316.55	0.7732	0.2268
319.35	0.7703	0.2297
322.55	0.7671	0.2329
327.55	0.7608	0.2392
330.85	0.7569	0.2431
334.05	0.7530	0.2470
336.35	0.7503	0.2497
338.95	0.7473	0.2527
344.55	0.7407	0.2593
349.45	0.7338	0.2662
351.25	0.7322	0.2678
354.75	0.7278	0.2722
358.25	0.2233	0.2767
359.85	0.7209	0.2791
364.35	0.7153	0.2847
367.75	0.7106	0.2894
370.35	0.7069	0.2931

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) 98% (starting purity), Chemical source not given, was an industrial product purified by dissolving in sodium hydroxide, followed by acidification, washing, and the recrystallized from water. Final purity was 99.8%.
(2) Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

Components:	**Original Measurements:**
(1) 4-Formylbenzoic acid; $C_8H_6O_3$; [619-66-9] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[84]D.-Q. Li, D.-Z. Liu, and F.-A. Wang, J. Chem. Eng. Data **46**, 172 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.25	0.8909	0.1091
300.15	0.8781	0.1219
306.35	0.8575	0.1425
308.85	0.8461	0.1539
312.65	0.8321	0.1679
317.85	0.8086	0.1914
321.65	0.7914	0.2086
322.45	0.7882	0.2118
326.05	0.7688	0.2312
329.15	0.7531	0.2469
331.95	0.7379	0.2621
335.05	0.7196	0.2804
337.45	0.7056	0.2944
338.65	0.6979	0.3021
340.95	0.6825	0.3175
341.75	0.6777	0.3223

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:
(1) 98% (starting purity), Chemical source not given, was an industrial product purified by dissolving in sodium hydroxide, followed by acidification, washing, and the recrystallized from water. Final purity was 99.8%.
(2) 99.0%, Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:
Temperature: ±0.05 K (estimated by compiler).
x_1: ±0.0005 or less.

46. Solubility of 2-Hydroxybenzoic Acid in Organic Solvents

46.1. Critical evaluation of experimental solubility data

There have been numerous studies[50,56,61,66,67,71,73,87,102,127,145–163] involving the solubility of 2-hydroxybenzoic acid (commonly referred to as salicylic acid) in organic solvents, particularly at 298 K. Most notably, Barra *et al.*[102] published solubility data for 2-hydroxybenzoic acid in two alkanes (heptane and cyclohexane), in one aromatic hydrocarbon (benzene), in one alkyl alkanoate (ethyl ethanoate), in one dialkyl ether (1,1′-oxybisethane) and one cyclic ether (1,4-dioxane), in two chloroalkanes (trichloromethane and 1,2-dichloroethane) and one chloroaromatic hydrocarbon (chlorobenzene), in seven alcohols (methanol, ethanol, 1-pentanol, 1-octanol, 1,2-ethanediol, 1,2-propanediol, and 1,2,3-propanetriol), in one alkanone (propanone) and one aromatic ketone (acetophenone), and in four miscellaneous organic solvents (ethanoic acid, propanoic acid, formamide, and *N*,*N*-dimethylformamide) as part of study directed towards calculating partial solubility parameters of sodium salts. The authors measured the solubility of a series of acid/sodium salt pairs. Replacement of the acidic proton by sodium ion was found to increase the dipolar and basic partial solubility parameters, whereas the dispersion parameter remained unchanged by the sodium for hydrogen substitution. Solubility data for 2-hydroxybenzoic acid in several alkane solvents (hexane, heptane, decane, dodecane, hexadecane, cyclohexane, and 2,2,4-trimethylpentane) were also determined by Fung and Higuchi.[146] De Fina *et al.*[151] measured solubilities of 2-hydroxybenzoic acid in two alkyl alkanoates (ethyl ethanoate and butyl ethanoate), in one dialkyl ether (1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in eight alcohols (1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, and 1-octanol), and three alkanones (propanone, butanone, and cyclohexanone). Matsuda *et al.*,[152] Shalmashi and Eliassi,[153] Gomaa *et al.*,[161] Ongley,[56] Lim *et al.*,[159] Fahkree *et al.*,[162] and Perlovich *et al.*[145] have also performed benzoic acid solubility measurements at 298 K.

The Abraham solvation parameter model can provide an indication of the quality of experimental solubility data for 2-hydroxybenzoic acid in a series of organic solvents of varying polarity and hydrogen bonding character. As discussed above, the evaluation will be restricted to those solvents where dimerization is not likely to occur and to solvents where 2-hydroxybenzoic acid does not form a solid solvate. This condition will limit the evaluation to primarily the alkyl alkanoates, dialkyl ethers, and alcohols. Numerical values of the solute descriptors for 2-hydroxybenzoic acid are known ($E = 0.900$, $S = 0.850$, $A = 0.730$, $B = 0.370$, and $V = 0.9904$), so that combination of these descriptors with the coefficients listed in Table 1 allows the prediction of $\log_{10}(c_{1,\mathrm{S}}/c_{1,\mathrm{W}})$. The molar solubility of molecular 2-hydroxybenzoic acid in water, $\log_{10} c_{1,\mathrm{W}} = -1.92$,[164] is available to convert the predicted $(c_{1,\mathrm{S}}/c_{1,\mathrm{W}})$ solubility ratios to $c_{1,\mathrm{S}}$ values. For carboxylic acid solutes, $c_{1,\mathrm{W}}$ corresponds to the aqueous solubility of the molecular, nonionized form of the solute.

The predicted molar solubilities of 2-hydroxybenzoic acid in methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-octanol, 2-propanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1,2-ethanediol, 1,1′-oxybisethane, tetrahydrofuran, 1,4-dioxane, ethyl ethanoate, butyl ethanoate, propanone, butanone, and cyclohexanone based on Eq. (20) are listed in the second column of Table 34. The numerical values represent outright solubility predictions in that none of the experimental data was used in the determination of the molecular solute descriptors. For comparison purposes, the measured mole fraction solubilities of 2-hydroxybenzoic acid, x_1, given in Secs. 46.2–46.10 were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 2-hydroxybenzoic acid is taken to be $V_{\mathrm{solute}} = 104\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$, which is larger than the value that other researchers have used. Sloan *et al.*[156] assumed a molar volume of 2-hydroxybenzoic acid of $V_1 = 93.9\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$. This latter value seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.1\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$, based on a molar mass of $106.12\ \mathrm{g\ mol}^{-1}$ and an experimental density of $1.0499\ \mathrm{g\ cm}^{-3}$ at 296 K. A molar volume on the order of $V_1 \approx 104\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$ would seem more realistic given the molecular structures of 2-hydroxybenzoic acid compared to benzaldehyde. To get an idea of how much error might be introduced in the mole fraction to molarity conversion, the mole fraction solubility of 2-hydroxybenzoic acid in ethyl ethanoate of $x_1 = 0.1383$ (Ref. 152) is converted into molar solubilities using both $V_1 = 93.9\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$ ($c_1 = 1.41\ \mathrm{mol\ dm}^{-3}$) and $V_1 \approx 104\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$ ($c_1 = 1.39\ \mathrm{mol\ dm}^{-3}$). Results of the computation suggest that any errors resulting from the estimation of 2-hydroxybenzoic acid's hypothetical subcooled liquid molar volume, V_{solute}, or the ideal molar volume approximation will have negligible effect of the calculated c_1 values because 2-hydroxybenzoic acid is not overly soluble in many of the solvents considered. From a mathematical standpoint, the $x_1^{\mathrm{exp}}V_{\mathrm{solute}}$ term contributes very little to the molar volumes of the saturated solutions.

TABLE 34. Comparison between observed and predicted molar solubilities of 2-hydroxybenzoic acid based on the Abraham model, Eq. (20)

Solvent	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10}$ c_1^{exp}	$\log_{10}$ c_1^{exp}	$\log_{10}$ c_1^{exp}	$\log_{10}$ c_1^{exp}
Methanol	0.514	0.430[a]			0.402[b]
Ethanol	0.574	0.237[a]		0.329[c]	0.347[b]
		0.296[d]	0.348[e]		
1-Propanol	0.443	0.256[e]	0.312[f]	0.262[g]	
2-Propanol	0.472		0.340[f]	0.253[g]	
1-Butanol	0.328	0.199[e]	0.243[f]		
2-Butanol	0.359		0.297[f]		
2-Methyl-1-propanol	0.268		0.180[f]		
2-Methyl-2-propanol	0.440		0.357[f]		
1-Pentanol	0.379	0.157[a]	0.174[f]	0.157[e]	
2-Pentanol	0.399				
3-Methyl-1-butanol	0.298				
1-Hexanol	0.307	0.114[e]			
1-Heptanol	0.240	0.072[e]			
1-Octanol	0.189	0.014[a]	0.165[f]	0.099[h]	
1-Decanol	0.176				
1,2-Ethanediol	0.180	0.152[a]			
1,1′-Oxybisethane	0.100	0.165[a]			
Tetrahydrofuran	0.712		0.609[f]		
1,4-Dioxane	0.353	0.514[a]	0.509[f]	0.460[b]	0.566[i]
Methyl ethanoate	0.008				
Ethyl ethanoate	0.146	0.091[a]	0.157[f]	0.143[c]	0.143[b]
Propyl ethanoate	0.068				
Butyl ethanoate	−0.010		0.025[f]		
Propanone	0.270	0.229[a]	0.359[f]	0.244[g]	0.376[j]
Butanone	0.240		0.300[f]		
Cyclohexanone	0.139		0.343[f]		

[a] Experimental value is taken from Barra *et al.*[102]
[b] Experimental value is taken from Matsuda *et al.*[152]
[c] Experimental value is taken from Shalmashi and Eliassi.[153]
[d] Experimental value is taken from Jouyban *et al.*[160]
[e] Experimental value is taken from Lim *et al.*[159]
[f] Experimental value is taken from De Fina *et al.*[151]
[g] Experimental value is taken from Fakhree *et al.*[162]
[h] Experimental value is taken from Perlovich *et al.*[145]
[i] Experimental value is taken from Peña *et al.*[157]
[j] Experimental value is taken from Marden and Dover.[149]

Solution models, like the Abraham solvation parameter model, prove useful in screening datasets for obvious outliers, particularly in cases where there are only one or two experimental data points for a given solute-solvent system. Such models are only able to identify those outliers, however, which fall outside of the model's expected predictive applicability. There is a sufficient number of data points for several of the solvents in Secs. 46.2–46.11 to compute a recommended value. The recommended mole fraction solubilities were calculated as an arithmetic average and are given in Table 35

TABLE 35. Recommended mole fraction solubilites for 2-hydroxybenzoic acid in selected solvents

Solvent	Recommended Value	Individual Values	Outliers
1,4-Dioxane	0.291	0.2945,[151] 0.2610,[152] 0.2978,[102] 0.3117 (Ref. 155)	
Tetrachloromethane	0.00306	0.00293,[67] 0.00291,[66] 0.00333 (Ref. 153)	0.00220 (Ref. 56)
Ethanol	0.141	0.1450,[152] 0.1386,[153] 0.1455,[159] 0.1397,[155] 0.1378,[154] 0.1369 (Ref. 71)	0.1100 (Ref. 102)
1-Butanol	0.155	0.1646,[151] 0.152,[127] 0.1484 (Ref. 159)	
1-Pentanol	0.157	0.1611,[151] 0.1547,[102] 0.1550 (Ref. 159)	

for the solvents that had three or more close solubility measurements. Included in the table are the individual mole fraction solubilities that went into the calculation, and any suspected outlier values. In the case of ethyl ethanoate, there are two different sets of three experimental values each [$x_1 = 0.1425$,[151] 0.1383,[152] and 0.1381 (Ref. 153)] and [$x_1 = 0.1152$,[154] 0.1223,[102] and 0.1136 (Ref. 135)], and one clear outlier value of $x_1 = 0.195$.[149] Since there is no way of knowing which of the two datasets is better, the recommended solubility in ethyl ethanoate of $x_1 = 0.128$ is calculated as the arithmetic average of all six experimental values [excluding the outlier). A similar situation occurs with 2-propanol, two different datasets of two values each, ($x_1 = 0.1320$ (Ref. 102) and 0.137 (Ref. 162)] and [$x_1 = 0.1817$ (Ref. 151) and 0.1892 (Ref. 149)]. Situations like this is why the criterion for making a recommendation was set at three or more data points that differed from each other by no more than approximately 15 relative percent.

There have been a few experimental studies examining the solubility of 2-hydroxybenzoic acid in different organic solvents as a function of temperature. Shalmashi and Eliassi[153] measured the solubility of 2-hydroxybenzoic acid in ethyl ethanoate, tetrachloromethane, and ethanol at eleven temperatures between 298 and 348 K using a gravimetric method. The authors described the observed mass fraction solubilities, w_1, with a simple linear relationship

$$\ln w_1 = A + B\,T, \tag{49}$$

where A and B are the intercept and slope of Eq. (49). The calculated values of A and B are tabulated in Table 36, along with the root-mean-square deviation defined by

$$\mathrm{RMSD} = \sqrt{\frac{\sum_i^N \left(w_i^{\mathrm{exp}} - w_i^{\mathrm{calc}}\right)^2}{N-1}}. \tag{50}$$

In Eq. (50), N represents the number of experimental values in the given data set, which in the present case would be 11. The two larger RMSDs of 0.0060 and 0.0082 occur in the 2-hydroxybenzoic acid + ethyl ethanoate and 2-hydroxybenzoic acid + ethanol systems, and correspond to approximately a 3% to 4% mean relative deviation.

Fakhree *et al.*[162] measured the solubility of 2-hydroxybenzoic acid in water, 1-propanol, 2-propanol, and propanone at five temperatures between 298 and 338 K, and in the three binary solvent mixtures containing water with each of the three organic compounds at 298 K. The authors described the variation in the molar solubility with temperature with a Modified Apelblat equation

$$\log_{10} c_1 = A + \frac{B}{T} + C \log_{10} T. \tag{51}$$

The calculated equation coefficients (A, B, and C), along with the mean percent relative deviation in molar concentration, are given in Table 37. Examination of the numerical entries in the last column of Table 37 reveals that the Apelblat type equation provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Lim *et al.*[159] examined the solubility behavior of 2-hydroxybenzoic acid in six neat 1-alkanols (ethanol through 1-heptanol) at temperatures from 278 to 318 K. The experimental data were correlated with the Non-Random Two-Liquid (NRTL), UNIQUAC, and Wilson models. Interaction coefficients calculated from the experimental solid-liquid equilibrium data provided a reasonably accurate mathematical description of the measured values. The mean absolute relative deviation between calculated and observed values was 0.475% (NRTL), 0.588% (Wilson model), and 0.429% (UNIQUAC model).

The experimental solubility data for 2-hydroxybenzoic acid in organic solvents are given in Secs. 46.2–46.11.

TABLE 36. Parameters of Eq. (49) for describing the solubility of 2-hydroxybenzoic acid in various organic solvents

Solvent	A	B	RMSD
Ethyl ethanoate[a]	−5.14	0.02	0.0060
Tetrachloromethane[a]	−18.59	0.04	0.0010
Ethanol[a]	−4.30	0.01	0.0082

[a] Values of the coefficients and the mean relative deviations were taken from Shalmashi and Eliassi.[153]

TABLE 37. Parameters of the Modified Apelblat-type equation for describing the solubility of 2-hydroxybenzoic acid in various organic solvents

Solvent	T/K	A	B	C	MRD (%)
1-Propanol[a]	298–338	1.514	−384.958	0	0.5
2-Propanol[a]	298–338	1.578	−396.006	0	0.8
Propanone[a]	298–338	−272.035	12249.4	93.438	0.1

[a] Values of the coefficients and mean relative deviation were taken from Fakhree *et al.*[162]

46.2. 2-Hydroxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Hexane; C_6H_{14}; [110-54-3]	[145]G. L. Perlovich, T. V. Volkova, and A. Bauer-Brandl, J. Pharm. Sci. **95**, 1448 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9996	0.000390
298	0.9995	0.000491
303	0.9994	0.000643
310	0.9990	0.000959
315	0.9988	0.00123

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration, the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:

(1) 99%, Sigma-Aldrich Inc., Oslo, Norway, no purification details provided.

(2) Analytical Reagent grade, SDS, Peypin, France, no purification details were provided.

Estimated Error:

Temperature: ±0.1 K.

x_2: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Hexane; C_6H_{14}; [110-54-3]	[146]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9995	0.00048

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Wrist-action shaker, constant-temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were allowed to equilibrate in a stoppered and sealed volumetric flask, which was continuously shaken (wrist-action shaken) for at least 24 h in a thermostated constant-temperature bath. An aliquot of saturated solution was transferred to a volumetric flask and diluted with trichloromethane. Concentrations were determined by spectrophotometric measurements at 306 nm.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, was recrystallized from hot water before use.

(2) Reagent grade, Chemical source not given, used as received.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Hexane; C_6H_{14}; [110-54-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9989	0.00111

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, no information provided concerning purification.

(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:

Temperature: No information given.

x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Heptane; C_7H_{16}; [142-82-5]	[146]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9995	0.00048

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Wrist-action shaker, constant-temperature bath, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a stoppered and sealed volumetric flask, which was continuously shaken (wrist-action shaken) for at least 24 h in a thermostated constant-temperature bath. An aliquot of saturated solution was transferred to a volumetric flask and diluted with trichloromethane. Concentrations were determined by spectrophotometric measurements at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from hot water before use.
(2) Reagent grade, Chemical source not given, was purified by passing the solvent through a column of silica gel and then distilled over sodium under reduced pressure.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Heptane; C_7H_{16}; [142-82-5]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9989	0.001116

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Heptane; C_7H_{16}; [142-82-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
365.4	0.985	0.0152
385.6	0.960	0.0395
397.9	0.923	0.0765
407.5	0.845	0.155
415.2	0.659	0.341
418.7	0.477	0.523
422.7	0.240	0.760

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 432.2 K.
(2) Purity not given, sample isolated from the resin of *Pinus sabiniana*, purified by treatment with sulfuric acid and nitric acid, and then distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	[146]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9996	0.00038

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Wrist-action shaker, constant-temperature bath, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a stoppered and sealed volumetric flask, which was continuously shaken (wrist-action shaken) for at least 24 h in a thermostated constant-temperature bath. An aliquot of saturated solution was transferred to a volumetric flask and diluted with trichloromethane. Concentrations were determined by spectrophotometric measurements at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from hot water before use.
(2) Reagent grade, Chemical source not given, was distilled from sodium under reduced pressure shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Decane; $C_{10}H_{22}$; [124-18-5]	[146]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9994	0.00062

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Wrist-action shaker, constant-temperature bath, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a stoppered and sealed volumetric flask, which was continuously shaken (wrist-action shaken) for at least 24 h in a thermostated constant-temperature bath. An aliquot of saturated solution was transferred to a volumetric flask and diluted with trichloromethane. Concentrations were determined by spectrophotometric measurements at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from hot water before use.
(2) Reagent grade, Chemical source not given, was purified by passing the solvent through a column of silica gel and then distilled over sodium under reduced pressure.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Dodecane; $C_{12}H_{26}$; [112-40-3]	[146]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9994	0.00064

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Wrist-action shaker, constant-temperature bath, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a stoppered and sealed volumetric flask, which was continuously shaken (wrist-action shaken) for at least 24 h in a thermostated constant-temperature bath. An aliquot of saturated solution was transferred to a volumetric flask and diluted with trichloromethane. Concentrations were determined by spectrophotometric measurements at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from hot water before use.
(2) Reagent grade, Chemical source not given, was purified by passing the solvent through a column of silica gel.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Hexadecane; $C_{16}H_{34}$; [544-76-3]	[146]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9990	0.00104

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Wrist-action shaker, constant-temperature bath, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a stoppered and sealed volumetric flask, which was continuously shaken (wrist-action shaken) for at least 24 h in a thermostated constant-temperature bath. An aliquot of saturated solution was transferred to a volumetric flask and diluted with trichloromethane. Concentrations were determined by spectrophotometric measurements at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from hot water before use.
(2) Reagent grade, Chemical source not given, was purified by passing the solvent through a column of silica gel and then distilled over sodium under reduced pressure.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[146]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9996	0.00043

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Wrist-action shaker, constant-temperature bath, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a stoppered and sealed volumetric flask, which was continuously shaken (wrist-action shaken) for at least 24 h in a thermostated constant-temperature bath. An aliquot of saturated solution was transferred to a volumetric flask and diluted with trichloromethane. Concentrations were determined by spectrophotometric measurements at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from hot water before use.
(2) Reagent grade, Chemical source not given, was distilled over phosphorous pentoxide shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 2.912$, which corresponds to a solubility of $c_1 = 0.00122$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9994	0.000551

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±10.0% (relative error, estimated by compiler).

46.3. 2-Hydroxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
317.5	0.989	0.0109
338.2	0.969	0.0305
371.7	0.871	0.129
387.7	0.717	0.283
404.7	0.496	0.504
413.2	0.289	0.711

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 432.2 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
284.9	0.9974	0.00259
291.4	0.9967	0.00326
303.7	0.9944	0.00557
307.8	0.9929	0.00708
309.8	0.9920	0.00802
322.6	0.9867	0.01328
337.4	0.9757	0.02428

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported as grams of solute per 100 g of solvent. Numerical values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator. Prior to titration, the solvent was removed by evaporation under reduced pressure.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[148] I. L. Krupatkin, J. Gen. Chem. USSR (Engl. Transl.) **26**, 3609 (1956).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
375.7	0.9711	0.0289
386.2	0.9501	0.0499
400.2	0.8832	0.1168
408.2	0.7963	0.2037
412.7	0.6670	0.3330
418.2	0.4311	0.5689
421.7	0.2383	0.7617

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined by a fusion method, which basically involves complete dissolution of the solid, followed by rapid solidification with vigorous stirring. The solid mass is then ground into smaller pieces. The melting point temperature of the mixture is then determined.

Source and Purity of Chemicals:
(1) Chemical Pure grade, Chemical source not given, no purification details were provided. Melting point temperature of sample is 428.2 K.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[56] P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.239$, which corresponds to a solubility of $c_1 = 0.0577 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[102] J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9945	0.00545

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[149] J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **39**, 1 (1917).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.995	0.00518

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance and a steam bath. Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 7 mg/ml of solution, which corresponds to a solubility of $c_1 = 0.0507$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9946	0.005441

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Methylbenzene; C_7H_8; [108-88-8]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9939	0.006052

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9934	0.006554

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

46.4. 2-Hydroxybenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8575	0.1425

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[152]H. Matsuda, K. Kaburagi, S. Matsumoto, K. Kurihara, K. Tochigi, and K. Tomono, J. Chem. Eng. Data **54**, 480 (2009).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8617	0.1383

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature water bath and high-performance liquid chromatograph with an uv detector.
Excess solute and solvent were allowed to equilibrate for 24 h in a constant-temperature thermostated water bath. Aliquots of saturated solutions were removed and filtered through a membrane filter of 0.45 μm pore size (Millipore, USA). Concentrations were determined by high-performance liquid chromatography equipped with an uv detector (254 nm detection). Benzene was added to the sample as an internal standard.

Source and Purity of Chemicals:
(1) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.
(2) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±6.2% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[153]A. Shalmashi and A. Eliassi, J. Chem. Eng. Data **53**, 199 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298	0.8619	0.1381
303	0.8491	0.1509
308	0.8356	0.1644
313	0.8227	0.1773
318	0.8097	0.1903
323	0.7965	0.2035
328	0.7845	0.2155
333	0.7707	0.2293
338	0.7570	0.2430
343	0.7431	0.2569
348	0.7281	0.2719

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetically stirred jacketed equilibrium cell, constant-temperature circulating water bath, and an analytical balance.
Excess solute and solvent were placed in a magnetically stirred jacketed equilibrium cell and allowed to equilibrate at constant temperature for 2 h with continuous stirring. After 2 h the stirring was discontinued and the suspended solid was allowed to settle to the lower portion of the equilibrium cell. An aliquot of the saturated solution was withdrawn by a warmed pipet and transferred to a weighed vial. The vial was tightly closed and weighed to determine the mass of the sample analyzed. The vial was then placed in an oven and the solvent was allowed to evaporate. The vial was reweighed, and the solubility calculated from the mass of the solid residue and sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized in the authors' department, dried under vacuum at 323 K for 8 h and then stored in a desiccator.
(2) Analytical grade, Merck Chemicals, Darmstadt, Germany, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8777	0.1223

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[154]M. A. Peña, B. Escalera, A. Reíllo, A. B. Sánchez, and P. Bustamante, J. Pharm. Sci. **98**, 1129 (2009).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.8915	0.1085
303	0.8781	0.1219
308	0.8707	0.1293
313	0.8671	0.1329

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a constant temperature-controlled shaking bath for four days at 313 K, and then one day at the lower temperatures. The authors used the same samples for all temperatures. The authors started with 313 K, and once the solution was saturated at the higher temperature they lowered the temperature for the next set of measurements. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 302 nm. The authors converted the molar solubilities to mole fractions using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Munich, Germany, was used as received.
(2) UV grade, Panreac, Monplet and Esteban, Barcelona, Spain, no purification details were provided.

Estimated Error:
Temperature: ±0.1.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[155]M. A. Peña, A. Reíllo, B. Escalera, and P. Bustamante, Int. J. Pharm. **321**, 155 (2006).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8864	0.1136

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent were allowed to equilibrate in a constant temperature-controlled shaking bath for at least five days. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 302 nm. The authors converted the molar solubilities to mole fractions using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Germany, no purification details were provided.
(2) Spectrophotometric grade, Panreac, Monplet and Esteban, Spain, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[149]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **39**, 1 (1917).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.805	0.195

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath.
Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 23 mg/ml of solution, which corresponds to a solubility of $c_1 = 0.167$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8637	0.1363

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 218.0 mg/ml, which corresponds to a molar solubility of $c_1 = 1.578$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Aldrich Chemical Company, UK, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.054.

Components:
(1) 2-Hydroxybenzoic acid;
$C_7H_6O_3$; [69-72-7]
(2) 1-Methylethyl tetradecanoate;
$C_{17}H_{34}O_2$; [110-27-0]

Original Measurements:
[156]K. B. Sloan, K. G. Siver, and S. A. M. Koch, J. Pharm. Sci. **75**, 744 (1986).

Variables:
T/K = 296

Prepared by:
W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 41.4 mg/ml, which corresponds to a solubility of $c_1 = 0.300$ mol dm^{-3}. The authors calculated a mole fraction solubility of $x_1 = 0.089$. The mole fraction solubility was calculated by the authors assuming a molar volume of 2-hydroxybenzoic acid of $V_1 = 93.9$ cm^3 mol^{-1}, which seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.1$ cm^3 mol^{-1}, based on a molar mass of 106.12 g mol^{-1} and an experimental density of 1.0499 g cm^{-3} at 296 K. A molar volume on the order of $V_1 \approx 104$ cm^3 mol^{-1} would seem more realistic given the molecular structures of 2-hydroxybenzoic acid compared to benzaldehyde.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer and an ultraviolet/visible spectrophotometer.
Solubility was determined by stirring an excess of solute in the solvent with a magnetic stirrer at ambient room temperature for 24 h in sealed flasks that were thermally insulated from the stirrer. The suspension was gravity filtered through Whatman #1 (qualitative) filter paper. The filtrate was then quantitatively diluted with methanol, and the absorbance of the diluted solution recorded at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.
(2) Purity not given, Givauden Corporation, Clifton, NJ, USA, used as received.

Estimated Error:
Temperature: ±1 K.
x_1: ±5% (relative error, estimated by compiler).

Components:
(1) 2-Hydroxybenzoic acid;
$C_7H_6O_3$; [69-72-7]
(2) 1-Methylethyl tetradecanoate;
$C_{17}H_{34}O_2$; [110-27-0]

Original Measurements:
[61]E. R. Cooper, J. Controlled Release **1**, 153 (1984).

Variables:
T/K = 295

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.925	0.075

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Fisher Scientific, Cincinnati, OH, USA, no purification details provided.
(2) Reagent grade, Wickhen Corporation, Huguenot, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

Components:
(1) 2-Hydroxybenzoic acid;
$C_7H_6O_3$; [69-72-7]
(2) 1-Methylethyl tetradecanoate;
$C_{17}H_{34}O_2$; [110-27-0]

Original Measurements:
[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).

Variables:
T/K = 305.2

Prepared by:
W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 66.0 mg/ml, which corresponds to a molar solubility of $c_1 = 0.478$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Croda Universal Ltd., no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.095.

46.5. 2-Hydroxybenzoic acid solubility data in ethers

Components:
(1) 2-Hydroxybenzoic acid;
$C_7H_6O_3$; [69-72-7]
(2) 1,1′-Oxybisethane;
$C_4H_{10}O$; [60-29-7]

Original Measurements:
[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8479	0.1521

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
T/K = 290	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 23.4 g/100 ml of solution, which corresponds to a molar concentration of 1.694 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
c_1: ±10% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9081	0.09185

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6358	0.3642

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7055	0.2945

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[152]H. Matsuda, K. Kaburagi, S. Matsumoto, K. Kurihara, K. Tochigi, and K. Tomono, J. Chem. Eng. Data **54**, 480 (2009).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7390	0.2610

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature water bath and high-performance liquid chromatograph with uv detector.
Excess solute and solvent were allowed to equilibrate for 24 h in a constant-temperature thermostated water bath. Aliquots of saturated solutions were removed and filtered through a membrane filter of 0.45 μm pore size (Millipore, USA). Concentrations were determined by high-performance liquid chromatography equipped with an uv detector (254 nm detection). Benzene was added to the sample as an internal standard.

Source and Purity of Chemicals:
(1) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.
(2) 99%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±6.2% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7022	0.2978

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[155]M. A. Peña, A. Reíllo, B. Escalera, and P. Bustamante, Int. J. Pharm. **321**, 155 (2006).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6883	0.3117

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent were allowed to equilibrate in a constant temperature-controlled shaking bath for at least five days. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 302 nm. The authors converted the molar solubilities to mole fractions using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Germany, no purification details were provided.
(2) Spectrophotometric grade, Panreac, Monplet and Esteban, Spain, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[157]M. A. Peña, P. Bustamante, B. Escalera, A. Reíllo, and J. M. Bosque-Sendra, J. Pharm. Biomed. Anal. **36**, 571 (2004).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
283	2.596
293	3.065
298	3.680
303	3.974
308	4.340
313	4.659

[a]c_1: molar solubility of the solute expressed in units of mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.
Excess solute and solvent were allowed first to equilibrate in a constant temperature-controlled shaking bath at 313 K, and then at the lower temperatures. The authors used the same samples for all temperatures. The authors started with 313 K, and once the solution was saturated at the higher temperature they lowered the temperature for the next set of measurements. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 298 nm.

Source and Purity of Chemicals:
(1) 99+%, Sigma Chemical Company, St. Louis, MO, USA, was used as received.
(2) 99.5+%, anhydrous, Panreac, Monplet and Esteban, Barcelona, Spain, no purification details were provided.

Estimated Error:
Temperature: ±0.1.
c_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 40 mg/ml of solution, which corresponds to a solubility of c_1 = 0.290 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±5% (relative error, estimated by compiler).

46.6. 2-Hydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.680$, which corresponds to a solubility of $c_1 = 0.209$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.157$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9985	0.001458

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2 mg/ml of solution, which corresponds to a solubility of c_1 = 0.0145 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9732	0.02679

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	[153]A. Shalmashi and A. Eliassi, J. Chem. Eng. Data **53**, 199 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298	0.9967	0.00333
303	0.9958	0.00420
308	0.9946	0.00544
313	0.9930	0.00702
318	0.9914	0.00856
323	0.9887	0.01134
328	0.9860	0.01396
333	0.9832	0.01681
338	0.9798	0.02002
343	0.9764	0.02363
348	0.9722	0.02778

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetically stirred jacketed equilibrium cell, constant-temperature circulating water bath, and an analytical balance.
Excess solute and solvent were placed in a magnetically stirred jacketed equilibrium cell and allowed to equilibrate at constant temperature for 2 h with continuous stirring. After 2 h the stirring was discontinued and the suspended solid was allowed to settle to the lower portion of the equilibrium cell. An aliquot of the saturated solution was withdrawn by a warmed pipet and transferred to a weighed vial. The vial was tightly closed and weighed to determine the mass of the sample analyzed. The vial was then placed in an oven and the solvent was allowed to evaporate. The vial was reweighed, and the solubility calculated from the mass of the solid residue and sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized in the authors' department, dried under vacuum at 323 K for 8 h and then stored in a desiccator.
(2) Analytical grade, Merck Chemicals, Darmstadt, Germany, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.644$, which corresponds to a solubility of $c_1 = 0.0227$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	[67]M. Davies and D. M. L. Griffiths, J. Chem. Soc. **1955**, 132.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9971	0.00293

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental solubility was determined by percolating the solvent at an adjustable rate through a column of solute in one limb of a U-shaped tube, a plug of cotton wool serving as support and filter. The saturated solution collects in the parallel arm and the whole assembly is immersed in a thermostat bath except for the stoppered ends. Samples of the saturated solutions were removed and titrated with standardized carbonate-free alkali using phenolphthalein as the indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9962	0.003803

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.030$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: No information was given.
x_1: ±4% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9924	0.00758

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.
x_1: ±5.0% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,1,2,2-Tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.131$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,1,1,2,2-Pentachloroethane; C_2HCl_5; [76-01-7]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.077$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Dichloroethene; $C_2H_2Cl_2$; isomer was not given	[86]D. H. Wester and A. Bruins, Pharm. Weekbl. **51**, 1443 (1914).
Variables: T/K = 288.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9947	0.00529

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were continuously shaken in a water bath at 303 K for 1 h. The solution was then transferred to a cellar which was maintained at a constant temperature of 288 K. The solution was allowed to equilibrate in the cellar for at least two days with repeated shaking. The concentration of the dissolved solute was determined; however, the analytical method was not described.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: Not enough information in paper to estimate an uncertainty.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Trichloroethene; C_2HCl_3; [79-06-1]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.110\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Trichloroethene; C_2HCl_3; [79-06-1]	[86]D. H. Wester and A. Bruins, Pharm. Weekbl. **51**, 1443 (1914).
Variables: T/K = 288.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9973	0.00268

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were continuously shaken in a water bath at 303 K for 1 h. The solution was then transferred to a cellar which was maintained at a constant temperature of 288 K. The solution was allowed to equilibrate in the cellar for at least two days with repeated shaking. The concentration of the dissolved solute was determined; however, the analytical method was not described.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: ±0.2 K.
x_1: Not enough information in paper to estimate an uncertainty.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Tetrachloroethene; C_2Cl_4; [127-18-4]	[66]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured molar solubility was $c_1 = 0.080 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were shaken in a thermostat at 298 K. After equilibrium was reached and the solid phase settled to the bottom of the container, an aliquot of the saturated clear solution was removed by pipet. The concentration of the solute in the saturated solution was determined by titration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9933	0.00670

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±5.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9921	0.007903

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

46.7. 2-Hydroxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Methanol; CH_4O; [67-56-1]	[152]H. Matsuda, K. Kaburagi, S. Matsumoto, K. Kurihara, K. Tochigi, and K. Tomono, J. Chem. Eng. Data **54**, 480 (2009).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8777	0.1223

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature water bath and high-performance liquid chromatograph with uv detector.
Excess solute and solvent were allowed to equilibrate for 24 h in a constant-temperature thermostated water bath. Aliquots of saturated solutions were removed and filtered through a membrane filter of 0.45 μm pore size (Millipore, USA). Concentrations were determined by high-performance liquid chromatography equipped with an uv detector (254 nm detection). Benzene was added to the sample as an internal standard.

Source and Purity of Chemicals:
(1) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.
(2) 99.8%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±6.2% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Methanol; CH_4O; [67-56-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8679	0.1321

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Methanol; CH_4O; [67-56-1]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 33.13 g/100 ml of solution, which corresponds to a molar concentration of 2.398 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Methanol; CH_4O; [67-56-1]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 299 mg/ml of solution, which corresponds to a solubility of c_1 = 2.16 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Methanol; CH_4O; [67-56-1]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8748	0.1252

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[152]H. Matsuda, K. Kaburagi, S. Matsumoto, K. Kurihara, K. Tochigi, and K. Tomono, J. Chem. Eng. Data **54**, 480 (2009).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8550	0.1450

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature water bath and high-performance liquid chromatograph with uv detector.
Excess solute and solvent were allowed to equilibrate for 24 h in a constant-temperature thermostated water bath. Aliquots of saturated solutions were removed and filtered through a membrane filter of 0.45 μm pore size (Millipore, USA). Concentrations were determined by high-performance liquid chromatography equipped with an uv detector (254 nm detection). Benzene was added to the sample as an internal standard.

Source and Purity of Chemicals:
(1) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.
(2) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±6.2% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[153]A. Shalmashi and A. Eliassi, J. Chem. Eng. Data **53**, 199 (2008).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298	0.8614	0.1386
303	0.8438	0.1562
308	0.8272	0.1728
313	0.8146	0.1854
318	0.8007	0.1993
323	0.7717	0.2283
328	0.7661	0.2339
333	0.7502	0.2498
338	0.7291	0.2709
343	0.7143	0.2857
348	0.6936	0.3064

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetically stirred jacketed equilibrium cell, constant-temperature circulating water bath, and an analytical balance.
Excess solute and solvent were placed in a magnetically stirred jacketed equilibrium cell and allowed to equilibrate at constant temperature for 2 h with continuous stirring. After 2 h the stirring was discontinued and the suspended solid was allowed to settle to the lower portion of the equilibrium cell. An aliquot of the saturated solution was withdrawn by a warmed pipet and transferred to a weighed vial. The vial was tightly closed and weighed to determine the mass of the sample analyzed. The vial was then placed in an oven and the solvent was allowed to evaporate. The vial was reweighed, and the solubility calculated from the mass of the solid residue and sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized in the authors' department, dried under vacuum at 323 K for 8 h and then stored in a desiccator.
(2) Analytical grade, Merck Chemicals, Darmstadt, Germany, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[159]J. Lim, S. Jang, H. K. Cho, M. S. Shin, and H. Kim, J. Chem. Thermodyn. **57**, 295 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.8916	0.1084
283.15	0.8831	0.1169
288.15	0.8745	0.1255
293.15	0.8642	0.1358
298.15	0.8545	0.1455
303.15	0.8434	0.1566
308.15	0.8303	0.1697
313.15	0.8179	0.1821
318.15	0.8031	0.1969

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer, drying oven and an analytical balance.
Excess solute and solvent were placed in 50-ml glass tubes and agitated with a magnetic stirrer at constant temperature for at least 48 h. A clear aliquot of the saturated solution was withdrawn using a syringe through a filter. The mass of the filtered clear solution was recorded. The sample was dried in a vacuum oven for at least seven days, and the mass of the solid residue recorded. The solution was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Samchen Pure Chemical Company, Seoul Korea, was used as received.
(2) 99.9%, Sigma Aldrich, St. Louis, MO, USA, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[160]A. Jouyban, V. Panahi-Azar, and F. Khonsari, J. Mol. Liq. **160**, 14 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
298.2	1.975
308.2	2.500
318.2	3.542
328.2	4.148

[a] c_1: molar solubility of the solute in units of moles per liter.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature incubator, temperature controlling system, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in sealed bottles and allowed to equilibrate at constant temperature in an incubator equipped with a temperature controlling system for at least two days. Solutions of the saturated solution were withdrawn and filtered using hydrophilic Durapore filters (0.45 μm). The filtered solutions were quantitatively diluted. Absorbances of the diluted solutions were measured. Concentrations of the diluted solutions were computed using a Beer-Law calibration curve based on measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:
(1) 98+%, Merck Chemical Company, Germany, was used as received.
(2) 99.5%, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
314.2	0.814	0.186
358.4	0.663	0.337
398.4	0.410	0.590

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 432.2 K.
(2) 99%, Chemical source not given, distilled over calcium oxide shortly before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[161]E. A. Gomaa, M. A. Mousa, and A. A. El-Khouly, Thermochim. Acta **86**, 351 (1985).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The authors' description regarding the experimental value is not clear. In the written text, the authors state that the concentration is in terms of the molal scale; however, in the footnote to Table 1 the unit is given as molal concentration/liter. The compiler has assumed that the numerical value is given in terms of molality, in which case the solubility is 2.874 mol/kg of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details are not definitive. Saturated solution was prepared by placing excess solute and solvent in test tubes. The sealed test tubes were allowed to equilibrate in a constant-temperature thermostated water bath for one week with shaking, followed by another day without shaking. Solubility was determined either gravimetrically or volumetrically. In the case of the gravimetric method, a 1 ml aliquot of saturated solution was evaporated to dryness in a small aluminum disk heated by an infrared lamp. In the volumetric method, 3–5 ml of the saturated solution was titrated with a standardized sodium hydroxide solution. The authors studied the solubility of three carboxylic acid solutes in seven different organic solvents, and did not specify which method was used for each solute-solvent pair.

Source and Purity of Chemicals:
(1) Analytical grade, Merck Chemical Company, Germany, no purification details were provided.
(2) Spectroscopic grade, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 28.19 g/100 ml of solution, which corresponds to a molar concentration of 2.041 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8900	0.1100

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
[155]M. A. Peña, A. Reíllo, B. Escalera, and P. Bustamante, Int. J. Pharm. **321**, 155 (2006).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8603	0.1397

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent were allowed to equilibrate in a constant temperature-controlled shaking bath for at least five days. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 302 nm. The authors converted the molar solubilities to mole fractions using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Germany, no purification details were provided.
(2) Spectrophotometric grade, Panreac, Monplet and Esteban, Spain, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
[154]M. A. Peña, B. Escalera, A. Reíllo, A. B. Sánchez, and P. Bustamante, J. Pharm. Sci. **98**, 1129 (2009).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.8652	0.1348
303	0.8595	0.1405
308	0.8515	0.1485
313	0.8395	0.1605

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.
Excess solute and solvent were allowed to equilibrate in a constant temperature-controlled shaking bath for four days at 313 K, and then one day at the lower temperatures. The authors used the same samples for all temperatures. The authors started with 313 K, and once the solution was saturated at the higher temperature they lowered the temperature for the next set of measurements. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 302 nm. The authors converted the molar solubilities to mole fractions using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Munich, Germany, was used as received.
(2) UV grade, Panreac, Monplet and Esteban, Barcelona, Spain, no purification details were provided.

Estimated Error:
Temperature: ±0.1.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[71]A. Seidell, Trans. Am. Electrochem. Soc. **13**, 319 (1908).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8631	0.1369

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a test tube and sealed with a rubber stopper. The test tube was attached to a rotating frame immersed in a constant-temperature water bath and revolved upon the axis parallel to the diameter of the test tube at the rate of approximately six revolutions per minute. The duration of the rotation was between four and seven days. At the end of the rotation period, the test tube was placed in an upright position in the bath with the stopper and a very small part of the test tube protruding from the bath, until the undissolved solid settled to the bottom of the test tube. A portion of the clear supernatant solution was withdrawn into a pipette having a cotton plug attached. The cotton plug served as a coarse filter. The concentration of the solution was determined by titration with standard alkali solution. The author determined the solubility of 2-hydroxybenzoic acid in several aqueous-alcohol solvent mixtures having ethanol concentrations between 0.00% and 99.8% by mass. The value for 100% ethanol was obtained from the curve of solubility versus alcohol concentration.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables: T/K = 305.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 368.2 mg/ml, which corresponds to a molar solubility of $c_1 = 2.666$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.033.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables: T/K = 303.8	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 377 mg/ml of solution, which corresponds to a solubility of $c_1 = 2.73$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8521	0.1479

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[162]M. A. A. Fakhree, S. Ahmadian, V. Panahi-Azar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **57**, 3303 (2012).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.868	0.132
308.2	0.850	0.150
318.2	0.837	0.163
328.2	0.821	0.179
338.2	0.805	0.195

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature oven, temperature controlling system, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in sealed bottles and allowed to equilibrate at constant temperature in an oven for three days. Samples were shaken manually three times per day to ensure that equilibrium had been achieved. Solutions of the saturated solution were withdrawn and filtered using hydrophilic Durapore filters (0.45 μm). The filtered solutions were quantitatively diluted with ethanol. Absorbances of the diluted solutions were measured at 304 nm. Concentrations of the diluted solutions were computed using a Beer-Law calibration curve based on measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:
(1) 99%, Merck Chemical Company, Germany, was used as received.
(2) 99.9%, Scharlau Chemie, Spain, was used as received.

Estimated Error:
Temperature: ±0.2 K to ±0.6 K; the higher temperatures have greater uncertainty.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8364	0.1636

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables: T/K = 293.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 22.25 g/100 ml of solution, which corresponds to a molar concentration of 1.611 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables: T/K = 303.8	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 287 mg/ml of solution, which corresponds to a solubility of $c_1 = 2.08$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[156]K. B. Sloan, K. G. Siver, and S. A. M. Koch, J. Pharm. Sci. **75**, 744 (1986).
Variables: T/K = 296	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 228 mg/ml, which corresponds to a solubility of $c_1 = 1.651$ mol dm^{-3}. The authors calculated a mole fraction solubility of $x_1 = 0.140$. The mole fraction solubility was calculated by the authors assuming a molar volume of 2-hydroxybenzoic acid of $V_1 = 93.9$ cm^3 mol^{-1}, which seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.1$ cm^3 mol^{-1}, based on a molar mass of 106.12 g mol^{-1} and an experimental density of 1.0499 g cm^{-3} at 296 K. A molar volume on the order of $V_1 \approx 104$ cm^3 mol^{-1} would seem more realistic given the molecular structures of 2-hydroxybenzoic acid compared to benzaldehyde.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer and an ultraviolet/visible spectrophotometer.
Solubility was determined by stirring an excess of solute in the solvent with a magnetic stirrer at ambient room temperature for 24 h in sealed flasks that were thermally insulated from the stirrer. The suspension was gravity filtered through Whatman #1 (qualitative) filter paper. The filtrate was then quantitatively diluted with methanol, and the absorbance of the diluted solution recorded at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.
(2) 99+%, Aldrich Chemical Company, used as received.

Estimated Error:
Temperature: ±1 K.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8562	0.1438

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[159]J. Lim, S. Jang, H. K. Cho, M. S. Shin, and H. Kim, J. Chem. Thermodyn. **57**, 295 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.8983	0.1017
283.15	0.8892	0.1108
288.15	0.8796	0.1204
293.15	0.8686	0.1314
298.15	0.8572	0.1428
303.15	0.8457	0.1543
308.15	0.8320	0.1680
313.15	0.8194	0.1806
318.15	0.8040	0.1960

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer, drying oven and an analytical balance.
Excess solute and solvent were placed in 50-ml glass tubes and agitated with a magnetic stirrer at constant temperature for at least 48 h. A clear aliquot of the saturated solution was withdrawn using a syringe through a filter. The mass of the filtered clear solution was recorded. The sample was dried in a vacuum oven for at least seven days, and the mass of the solid residue recorded. The solution was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Samchen Pure Chemical Company, Seoul Korea, was used as received.
(2) 99.9%, Sigma Aldrich, St. Louis, MO, USA, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2-Propanol; C_3H_8O; [67-63-0]	[162]M. A. A. Fakhree, S. Ahmadian, V. Panahi-Azar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **57**, 3303 (2012).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.856	0.144
308.2	0.839	0.161
318.2	0.827	0.173
328.2	0.805	0.195
338.2	0.786	0.214

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature oven, temperature controlling system, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in sealed bottles and allowed to equilibrate at constant temperature in an oven for three days. Samples were shaken manually three times per day to ensure that equilibrium had been achieved. Solutions of the saturated solution were withdrawn and filtered using hydrophilic Durapore filters (0.45 μm). The filtered solutions were quantitatively diluted with ethanol. Absorbances of the diluted solutions were measured at 304 nm. Concentrations of the diluted solutions were computed using a Beer-Law calibration curve based on measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:
(1) 99%, Merck Chemical Company, Germany, was used as received.
(2) 99.9%, Scharlau Chemie, Spain, was used as received.

Estimated Error:
Temperature: ±0.2 K to ±0.6 K; the higher temperatures have greater uncertainty.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2-Propanol; C_3H_8O; [67-63-0]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8211	0.1789

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8354	0.1646

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.2	0.852	0.148
311.2	0.821	0.179
358.8	0.661	0.339
394.8	0.329	0.671

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 432.2 K.
(2) Purity not given, Chemical source not given, fractionated and distilled several times before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 283.7 mg/ml, which corresponds to a molar solubility of $c_1 = 2.053$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.03 (estimated by compiler, value in the paper seemed too small given the analytical method).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 251 mg/ml of solution, which corresponds to a solubility of $c_1 = 1.82$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8412	0.1588

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[159]J. Lim, S. Jang, H. K. Cho, M. S. Shin, and H. Kim, J. Chem. Thermodyn. **57**, 295 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.8937	0.1063
283.15	0.8842	0.1158
288.15	0.8745	0.1255
293.15	0.8633	0.1367
298.15	0.8516	0.1484
303.15	0.8403	0.1597
308.15	0.8264	0.1736
313.15	0.8137	0.1863
318.15	0.7988	0.2012

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer, drying oven and an analytical balance.
Excess solute and solvent were placed in 50-ml glass tubes and agitated with a magnetic stirrer at constant temperature for at least 48 h. A clear aliquot of the saturated solution was withdrawn using a syringe through a filter. The mass of the filtered clear solution was recorded. The sample was dried in a vacuum oven for at least seven days, and the mass of the solid residue recorded. The solution was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Samchen Pure Chemical Company, Seoul Korea, was used as received.
(2) 99.7%, Sigma Aldrich, St. Louis, MO, USA, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8131	0.1869

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[151] K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8570	0.1430

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[151] K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7807	0.2193

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[151] K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8389	0.1611

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8453	0.1547

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[159]J. Lim, S. Jang, H. K. Cho, M. S. Shin, and H. Kim, J. Chem. Thermodyn. **57**, 295 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.8872	0.1128
283.15	0.8773	0.1227
288.15	0.8677	0.1323
293.15	0.8560	0.1440
298.15	0.8450	0.1550
303.15	0.8337	0.1663
308.15	0.8198	0.1802
313.15	0.8081	0.1919
318.15	0.7941	0.2059

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer, drying oven and an analytical balance.
Excess solute and solvent were placed in 50-ml glass tubes and agitated with a magnetic stirrer at constant temperature for at least 48 h. A clear aliquot of the saturated solution was withdrawn using a syringe through a filter. The mass of the filtered clear solution was recorded. The sample was dried in a vacuum oven for at least seven days, and the mass of the solid residue recorded. The solution was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Samchen Pure Chemical Company, Seoul Korea, was used as received.
(2) 99%, Sigma Aldrich, St. Louis, MO, USA, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[159]J. Lim, S. Jang, H. K. Cho, M. S. Shin, and H. Kim, J. Chem. Thermodyn. **57**, 295 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.8837	0.1163
283.15	0.8731	0.1269
288.15	0.8633	0.1367
293.15	0.8542	0.1458
298.15	0.8416	0.1584
303.15	0.8309	0.1691
308.15	0.8180	0.1820
313.15	0.8050	0.1950
318.15	0.7911	0.2089

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer, drying oven and an analytical balance.
Excess solute and solvent were placed in 50-ml glass tubes and agitated with a magnetic stirrer at constant temperature for at least 48 h. A clear aliquot of the saturated solution was withdrawn using a syringe through a filter. The mass of the filtered clear solution was recorded. The sample was dried in a vacuum oven for at least seven days, and the mass of the solid residue recorded. The solution was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Samchen Pure Chemical Company, Seoul Korea, was used as received.
(2) 99%, Sigma Aldrich, St. Louis, MO, USA, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[159]J. Lim, S. Jang, H. K. Cho, M. S. Shin, and H. Kim, J. Chem. Thermodyn. **57**, 295 (2013).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.15	0.8828	0.1172
283.15	0.8720	0.1280
288.15	0.8623	0.1377
293.15	0.8515	0.1485
298.15	0.8396	0.1604
303.15	0.8286	0.1714
308.15	0.8154	0.1846
313.15	0.8031	0.1969
318.15	0.7898	0.2102

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility data were reported as mass fractions. The mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer, drying oven and an analytical balance.
Excess solute and solvent were placed in 50-ml glass tubes and agitated with a magnetic stirrer at constant temperature for at least 48 h. A clear aliquot of the saturated solution was withdrawn using a syringe through a filter. The mass of the filtered clear solution was recorded. The sample was dried in a vacuum oven for at least seven days, and the mass of the solid residue recorded. The solution was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Samchen Pure Chemical Company, Seoul Korea, was used as received.
(2) 98%, Tokyo Chemical Industry, Tokyo, Japan, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7857	0.2143

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8452	0.1548

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[145]G. L. Perlovich, T. V. Volkova, and A. Bauer-Brandl, J. Pharm. Sci. **95**, 1448 (2006).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.824	0.176
298	0.814	0.186
303	0.794	0.206
310	0.765	0.235
315	0.748	0.252

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration, the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich Inc., Oslo, Norway, no purification details provided.
(2) Analytical Reagent grade, Sigma-Aldrich Inc., no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_2: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables: T/K = 305.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 186.1 mg/ml, which corresponds to a molar solubility of $c_1 = 1.347$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.02.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[156]K. B. Sloan, K. G. Siver, and S. A. M. Koch, J. Pharm. Sci. **75**, 744 (1986).
Variables: T/K = 296	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 145 mg/ml, which corresponds to a solubility of $c_1 = 1.050\ \text{mol dm}^{-3}$. The authors calculated a mole fraction solubility of $x_1 = 0.157$. The mole fraction solubility was calculated by the authors assuming a molar volume of 2-hydroxybenzoic acid of $V_1 = 93.9\ \text{cm}^3\ \text{mol}^{-1}$, which seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.1\ \text{cm}^3\ \text{mol}^{-1}$, based on a molar mass of $106.12\ \text{g mol}^{-1}$ and an experimental density of $1.0499\ \text{g cm}^{-3}$ at 296 K. A molar volume on the order of $V_1 \approx 104\ \text{cm}^3\ \text{mol}^{-1}$ would seem more realistic given the molecular structures of 2-hydroxybenzoic acid compared to benzaldehyde.

Auxiliary Information

Method/Apparatus/Procedure:
Magnetic stirrer and an ultraviolet/visible spectrophotometer.
Solubility was determined by stirring an excess of solute in the solvent with a magnetic stirrer at ambient room temperature for 24 h in sealed flasks that were thermally insulated from the stirrer. The suspension was gravity filtered through Whatman #1 (qualitative) filter paper. The filtrate was then quantitatively diluted with methanol, and the absorbance of the diluted solution recorded at 306 nm.

Source and Purity of Chemicals:
(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.
(2) 99+%, Aldrich Chemical Company, used as received.

Estimated Error:
Temperature: ±1 K.
x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables: T/K = 305.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 136.9 mg/ml, which corresponds to a molar solubility of $c_1 = 0.991\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific, UK, no purification details were provided.
(2) Purity not given, Fisher Scientific, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.02.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables: T/K = 303.8	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 217 mg/ml of solution, which corresponds to a solubility of $c_1 = 1.571\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Benzenemethanol; C_7H_8O; [100-51-6]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables: T/K = 303.8	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 203 mg/ml of solution, which corresponds to a solubility of $c_1 = 1.47\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9149	0.08509

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables: T/K = 303.8	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 42 mg/ml of solution, which corresponds to a solubility of $c_1 = 0.304$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8864	0.1136

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[160]A. Jouyban, V. Panahi-Azar, and F. Khonsari, J. Mol. Liq. **160**, 14 (2011).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
298.2	1.592
308.2	2.144
318.2	3.061
328.2	3.382

[a] c_1: molar solubility of the solute in units of moles per liter.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature incubator, temperature controlling system, and ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in sealed bottles and allowed to equilibrate at constant temperature in an incubator equipped with a temperature controlling system for at least two days. Solutions of the saturated solution were withdrawn and filtered using hydrophilic Durapore filters (0.45 μm). The filtered solutions were quantitatively diluted. Absorbances of the diluted solutions were measured. Concentrations of the diluted solutions were computed using a Beer-Law calibration curve based on measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:

(1) 98+%, Merck Chemical Company, Germany, was used as received.

(2) 99.5%, Merck Chemical Company, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

c_1: ±3% (relative error).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[73]M. Dias, S. L. Raghavan, and J. Hadgraft, Int. J. Pharm. **216**, 51 (2001).
Variables: T/K = 305.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 192.8 mg/ml, which corresponds to a molar solubility of $c_1 = 1.396$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:

(1) Purity not given, Fisher Scientific, UK, no purification details were provided.

(2) Purity not given, Fisher Scientific, no purification details were provided.

Estimated Error:

Temperature: Insufficient experimental details to estimate.

c_1: ±0.14.

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables: T/K = 303.8	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 118 mg/ml of solution, which corresponds to a solubility of $c_1 = 0.854$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

c_1: ±5% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[156]K. B. Sloan, K. G. Siver, and S. A. M. Koch, J. Pharm. Sci. **75**, 744 (1986).
Variables: T/K = 296	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 207 mg/ml, which corresponds to a solubility of $c_1 = 1.499$ mol dm^{-3}. The authors calculated a mole fraction solubility of $x_1 = 0.116$. The mole fraction solubility was calculated by the authors assuming a molar volume of 2-hydroxybenzoic acid of $V_1 = 93.9$ cm^3 mol^{-1}, which seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.1$ cm^3 mol^{-1}, based on a molar mass of 106.12 g mol^{-1} and an experimental density of 1.0499 g cm^{-3} at 296 K. A molar volume on the order of $V_1 \approx 104$ cm^3 mol^{-1} would seem more realistic given the molecular structures of 2-hydroxybenzoic acid compared to benzaldehyde.

Auxiliary Information

Method/Apparatus/Procedure:

Magnetic stirrer and an ultraviolet/visible spectrophotometer.

Solubility was determined by stirring an excess of solute in the solvent with a magnetic stirrer at ambient room temperature for 24 h in sealed flasks that were thermally insulated from the stirrer. The suspension was gravity filtered through Whatman #1 (qualitative) filter paper. The filtrate was then quantitatively diluted with methanol, and the absorbance of the diluted solution recorded at 306 nm.

Source and Purity of Chemicals:

(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

(2) 99+%, Aldrich Chemical Company, used as received.

Estimated Error:

Temperature: ±1 K.

x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[61]E. R. Cooper, J. Controlled Release **1**, 153 (1984).
Variables	**Prepared by:**
T/K = 295	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.872	0.128

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:

(1) Reagent grade, Fisher Scientific, Cincinnati, OH, USA, no purification details provided.

(2) Reagent grade, J.T. Baker Chemical Company, Phillipsburg, NJ, USA, no purification details provided.

Estimated Error:

Temperature: No information given.

x_1: No information given.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2,3-Propanetriol (Glycerol); $C_3H_8O_3$; [60-29-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9253	0.07465

[a]x_2: mole fraction of component 2 in the saturated solution.

[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.

(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2,3-Propanetriol (Glycerol); $C_3H_8O_3$; [60-29-7]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 15 mg/ml of solution, which corresponds to a solubility of $c_1 = 0.109$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1,2,3-Propanetriol (Glycerol); $C_3H_8O_3$; [56-81-5]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 24.99 mg/ml, which corresponds to a molar solubility of $c_1 = 0.181$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, ICN Biochemicals, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.022.

46.8. 2-Hydroxybenzoic acid solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 425 mg/ml of solution, which corresponds to a solubility of $c_1 = 3.08$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

46.9. 2-Hydroxybenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[162]M. A. A. Fakhree, S. Ahmadian, V. Panahi-Azar, W. E. Acree, Jr., and A. Jouyban, J. Chem. Eng. Data **57**, 3303 (2012).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.863	0.137
308.2	0.861	0.139
318.2	0.844	0.156
328.2	0.804	0.196

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant temperature oven, temperature controlling system, and ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in sealed bottles and allowed to equilibrate at constant temperature in an oven for three days. Samples were shaken manually three times per day to ensure that equilibrium had been achieved. Solutions of the saturated solution were withdrawn and filtered using hydrophilic Durapore filters (0.45 μm). The filtered solutions were quantitatively diluted with ethanol. Absorbances of the diluted solutions were measured at 304 nm. Concentrations of the diluted solutions were computed using a Beer-Law calibration curve based on measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:

(1) 99%, Merck Chemical Company, Germany, was used as received.
(2) 99.5%, Scharlau Chemie, Spain, was used as received.

Estimated Error:

Temperature: ±0.2 K to ±0.6 K, the higher temperatures have greater uncertainty.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8183	0.1817

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:

(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.9+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:

Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8680	0.1320

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 29.44 g/100 ml of solution, which corresponds to a molar concentration of 2.131 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[150]A. N. Paruta, B. J. Sciarrone, and N. G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
T/K = 303.8	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 381 mg/ml of solution, which corresponds to a solubility of $c_1 = 2.76$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in 15-ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a constant-temperature water bath and allowed to equilibrate for 24 h. An aliquot of the saturated solution was withdrawn from the vial with a pipet fitted with a glass wool filtering plug. The solubility was determined by titration using a freshly prepared sodium hydroxide solution. The endpoint of the titration was detected with phenolphthalein.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[50]P. G. Desai and A. M. Patel, J. Ind. Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
T/K = 301.2	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8094	0.1906

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[149]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **39**, 1 (1917).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8108	0.1892

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Experimental solubility data were given as grams of solute per 100 g of solvent. Mole fraction solubility was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath.
Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±10.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
T/K = 296	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 31.3 g/100 ml of solution, which corresponds to a molar concentration of 2.266 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
c_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Butanone; C_4H_8O; [78-93-3]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8148	0.1852

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.5+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Butanone; C_4H_8O; [78-93-3]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 23.56 g/100 ml of solution, which corresponds to a molar concentration of 1.706 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 2-Pentanone; $C_5H_{10}O$; [107-87-9]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 20.92 g/100 ml of solution, which corresponds to a molar concentration of 1.515 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]	[151]K. M. De Fina, T. L. Sharp, L. E. Roy, and W. E. Acree, Jr., J. Chem. Eng. Data **44**, 1262 (1999).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7699	0.2301

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 304 nm.

Source and Purity of Chemicals:
(1) 99+%, ACS Reagent grade, Aldrich Chemical Company, Milwaukee, WI, USA, was dried for several hours at 353 K before use and used without further purification.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Acetophenone; C_8H_8O; [98-86-2]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8473	0.1527

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

46.10. 2-Hydroxybenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[160]A. Jouyban, V. Panahi-Azar, and F. Khonsari, J. Mol. Liq. **160**, 14 (2011).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	c_1[a]
298.2	3.934
308.2	5.749
318.2	8.296
328.2	10.258

[a] c_1: molar solubility of the solute in units of moles per liter.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature incubator, temperature controlling system, and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in sealed bottles and allowed to equilibrate at constant temperature in an incubator equipped with a temperature controlling system for at least two days. Solutions of the saturated solution were withdrawn and filtered using hydrophilic Durapore filters (0.45 μm). The filtered solutions were quantitatively diluted. Absorbances of the diluted solutions were measured. Concentrations of the diluted solutions were computed using a Beer-Law calibration curve based on measured absorbances for standard solutions of known concentration.

Source and Purity of Chemicals:
(1) 98+%, Merck Chemical Company, Germany, was used as received.
(2) 99.5%, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
c_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[161]E. A. Gomaa, M. A. Mousa, and A. A. El-Khouly, Thermochim. Acta **86**, 351 (1985).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The authors' description regarding the experimental value is not clear. In the written text, the authors state that the concentration is in terms of the molal scale; however, in the footnote to Table 1 the unit is given as molal concentration/liter. The compiler has assumed that the numerical value is given in terms of molality, in which case the solubility is 5.526 mol/kg of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details are not definitive. Saturated solution was prepared by placing excess solute and solvent in test tubes. The sealed test tubes were allowed to equilibrate in a constant-temperature thermostated water bath for one week with shaking, followed by another day without shaking. Solubility was determined either gravimetrically or volumetrically. In the case of the gravimetric method, a 1 ml aliquot of saturated solution was evaporated to dryness in a small aluminum disk heated by an infrared lamp. In the volumetric method, 3–5 ml of the saturated solution was titrated with a standardized sodium hydroxide solution. The authors studied the solubility of three carboxylic acid solutes in seven different organic solvents, and did not specify which method was used for each solute-solvent pair.

Source and Purity of Chemicals:
(1) Analytical grade, Merck Chemical Company, Germany, no purification details were provided.
(2) Spectroscopic grade, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[161]E. A. Gomaa, M. A. Mousa, and A. A. El-Khouly, Thermochim. Acta **86**, 351 (1985).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The authors' description regarding the experimental value is not clear. In the written text, the authors state that the concentration is in terms of the molal scale; however, in the footnote to Table 1 the unit is given as molal concentration/liter. The compiler has assumed that the numerical value is given in terms of molality, in which case the solubility is 0.283 mol/kg of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details are not definitive. Saturated solution was prepared by placing excess solute and solvent in test tubes. The sealed test tubes were allowed to equilibrate in a constant-temperature thermostated water bath for one week with shaking, followed by another day without shaking. Solubility was determined either gravimetrically or volumetrically. In the case of the gravimetric method, a 1 ml aliquot of saturated solution was evaporated to dryness in a small aluminum disk heated by an infrared lamp. In the volumetric method, 3–5 ml of the saturated solution was titrated with a standardized sodium hydroxide solution. The authors studied the solubility of three carboxylic acid solutes in seven different organic solvents, and did not specify which method was used for each solute-solvent pair.

Source and Purity of Chemicals:
(1) Analytical grade, Merck Chemical Company, Germany, no purification details were provided.
(2) Spectroscopic grade, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[161]E. A. Gomaa, M. A. Mousa, and A. A. El-Khouly, Thermochim. Acta **86**, 351 (1985).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The authors' description regarding the experimental value is not clear. In the written text, the authors state that the concentration is in terms of the molal scale; however, in the footnote to Table 1 the unit is given as molal concentration/liter. The compiler has assumed that the numerical value is given in terms of molality, in which case the solubility is 4.911 mol/kg of solvent.

Auxiliary Information

Method/Apparatus/Procedure:

Experimental details are not definitive. Saturated solution was prepared by placing excess solute and solvent in test tubes. The sealed test tubes were allowed to equilibrate in a constant-temperature thermostated water bath for one week with shaking, followed by another day without shaking. Solubility was determined either gravimetrically or volumetrically. In the case of the gravimetric method, a 1 ml aliquot of saturated solution was evaporated to dryness in a small aluminum disk heated by an infrared lamp. In the volumetric method, 3–5 ml of the saturated solution was titrated with a standardized sodium hydroxide solution. The authors studied the solubility of three carboxylic acid solutes in seven different organic solvents, and did not specify which method was used for each solute-solvent pair.

Source and Purity of Chemicals:

(1) Analytical grade, Merck Chemical Company, Germany, no purification details were provided.

(2) Spectroscopic grade, Merck Chemical Company, no purification details were provided.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Formamide; CH_3NO; [75-12-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9574	0.04264

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.

(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Formamide; CH_3NO; [75-12-7]	[156]K. B. Sloan, K. G. Siver, and S. A. M. Koch, J. Pharm. Sci. **75**, 744 (1986).
Variables:	**Prepared by:**
T/K = 296	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 145 mg/ml, which corresponds to a solubility of $c_1 = 1.050$ mol dm^{-3}. The authors calculated a mole fraction solubility of $x_1 = 0.045$. The mole fraction solubility was calculated by the authors assuming a molar volume of 2-hydroxybenzoic acid of $V_1 = 93.9$ cm^3 mol^{-1}, which seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.1$ cm^3 mol^{-1}, based on a molar mass of 106.12 g mol^{-1} and an experimental density of 1.0499 g cm^{-3} at 296 K. A molar volume on the order of $V_1 \approx 104$ cm^3 mol^{-1} would seem more realistic given the molecular structures of 2-hydroxybenzoic acid compared to benzaldehyde.

Auxiliary Information

Method/Apparatus/Procedure:

Magnetic stirrer and an ultraviolet/visible spectrophotometer.

Solubility was determined by stirring an excess of solute in the solvent with a magnetic stirrer at ambient room temperature for 24 h in sealed flasks that were thermally insulated from the stirrer. The suspension was gravity filtered through Whatman #1 (qualitative) filter paper. The filtrate was then quantitatively diluted with methanol, and the absorbance of the diluted solution recorded at 306 nm.

Source and Purity of Chemicals:

(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

(2) 99+%, Aldrich Chemical Company, used as received.

Estimated Error:

Temperature: ±1 K.

x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) *N*-Methylformamide; C_2H_5NO; [123-39-7]	[161]E. A. Gomaa, M. A. Mousa, and A. A. El-Khouly, Thermochim. Acta **86**, 351 (1985).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The authors' description regarding the experimental value is not clear. In the written text, the authors state that the concentration is in terms of the molal scale; however, in the footnote to Table 1 the unit is given as molal concentration/liter. The compiler has assumed that the numerical value is given in terms of molality, in which case the solubility is 3.807 mol/kg of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details are not definitive. Saturated solution was prepared by placing excess solute and solvent in test tubes. The sealed test tubes were allowed to equilibrate in a constant-temperature thermostated water bath for one week with shaking, followed by another day without shaking. Solubility was determined either gravimetrically or volumetrically. In the case of the gravimetric method, a 1 ml aliquot of saturated solution was evaporated to dryness in a small aluminum disk heated by an infrared lamp. In the volumetric method, 3–5 ml of the saturated solution was titrated with a standardized sodium hydroxide solution. The authors studied the solubility of three carboxylic acid solutes in seven different organic solvents, and did not specify which method was used for each solute-solvent pair.

Source and Purity of Chemicals:
(1) Analytical grade, Merck Chemical Company, Germany, no purification details were provided.
(2) Spectroscopic grade, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[161]E. A. Gomaa, M. A. Mousa, and A. A. El-Khouly, Thermochim. Acta **86**, 351 (1985).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The authors' description regarding the experimental value is not clear. In the written text, the authors state that the concentration is in terms of the molal scale; however, in the footnote to Table 1 the unit is given as molal concentration/liter. The compiler has assumed that the numerical value is given in terms of molality, in which case the solubility is 4.459 mol/kg of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details are not definitive. Saturated solution was prepared by placing excess solute and solvent in test tubes. The sealed test tubes were allowed to equilibrate in a constant-temperature thermostated water bath for one week with shaking, followed by another day without shaking. Solubility was determined either gravimetrically or volumetrically. In the case of the gravimetric method, a 1 ml aliquot of saturated solution was evaporated to dryness in a small aluminum disk heated by an infrared lamp. In the volumetric method, 3–5 ml of the saturated solution was titrated with a standardized sodium hydroxide solution. The authors studied the solubility of three carboxylic acid solutes in seven different organic solvents, and did not specify which method was used for each solute-solvent pair.

Source and Purity of Chemicals:
(1) Analytical grade, Merck Chemical Company, Germany, no purification details were provided.
(2) Spectroscopic grade, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6160	0.3840

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[161]E. A. Gomaa, M. A. Mousa, and A. A. El-Khouly, Thermochim. Acta **86**, 351 (1985).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The authors' description regarding the experimental value is not clear. In the written text, the authors state that the concentration is in terms of the molal scale; however, in the footnote to Table 1 the unit is given as molal concentration/liter. The compiler has assumed that the numerical value is given in terms of molality, in which case the solubility is 0.621 mol/kg of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental details are not definitive. Saturated solution was prepared by placing excess solute and solvent in test tubes. The sealed test tubes were allowed to equilibrate in a constant-temperature thermostated water bath for one week with shaking, followed by another day without shaking. Solubility was determined either gravimetrically or volumetrically. In the case of the gravimetric method, a 1 ml aliquot of saturated solution was evaporated to dryness in a small aluminum disk heated by an infrared lamp. In the volumetric method, 3–5 ml of the saturated solution was titrated with a standardized sodium hydroxide solution. The authors studied the solubility of three carboxylic acid solutes in seven different organic solvents, and did not specify which method was used for each solute-solvent pair.

Source and Purity of Chemicals:
(1) Analytical grade, Merck Chemical Company, Germany, no purification details were provided.
(2) Spectroscopic grade, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	[50]P. G. Desai and A. M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables: T/K = 301.2	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9749	0.02509

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were placed in a glass flask which was kept revolving on a wheel in an air thermostat for two days. After two days of equilibration, the solution was filtered. To minimize absorption of the solute onto the filter paper, a 100 ml portion of fresh saturated solution was first filtered through the paper before filtering the sample to be analyzed. An aliquot of the filtrate was titrated with barium hydroxide using phenolphthalein as the endpoint indictor. The barium hydroxide titrant was previously standardized against a solution of succinic acid.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, no information provided concerning purification.
(2) Purity not given, Chemical source not specified, no information provided concerning purification.

Estimated Error:
Temperature: No information given.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9402	0.05979

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:
(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.
(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanoic acid; $C_3H_6O_2$; [79-09-4]	[102]J. Barra, M.-A. Peña, and P. Bustamante, Eur. J. Pharm. Sci. **10**, 153 (2000).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9339	0.06614

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, analytical balance, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in a flask and allowed to equilibrate for several days at constant temperature. The solid phase was removed by filtration, and the clear solution was diluted quantitatively with 96% ethanol. The concentration of the diluted solution was determined by spectrophotometric measurement at the wavelength of maximum absorption. In instances where the solvent interfered with the spectrophotometric determination, the samples were evaporated to dryness and the residue diluted with 96% ethanol.

Source and Purity of Chemicals:

(1) Purity not given, Sigma Chemical Company, USA, no purification details were provided.

(2) Spectrophotometric or Analytical grade, Chemical source not specified, no purification details were provided.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 9(Z)-Octadecenoic acid (Oleic acid); $C_{18}H_{34}O_2$; [112-80-1]	[156]K. B. Sloan, K. G. Siver, and S. A. M. Koch, J. Pharm. Sci. **75**, 744 (1986).
Variables:	**Prepared by:**
T/K = 296	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 30.3 mg/ml, which corresponds to a solubility of $c_1 = 0.219$ mol dm^{-3}. The authors calculated a mole fraction solubility of $x_1 = 0.066$. The mole fraction solubility was calculated by the authors assuming a molar volume of 2-hydroxybenzoic acid of $V_1 = 93.9$ cm^3 mol^{-1}, which seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.1$ cm^3 mol^{-1}, based on a molar mass of 106.12 g mol^{-1} and an experimental density of 1.0499 g cm^{-3} at 296 K. A molar volume on the order of $V_1 \approx 104$ cm^3 mol^{-1} would seem more realistic given the molecular structures of 2-hydroxybenzoic acid compared to benzaldehyde.

Auxiliary Information

Method/Apparatus/Procedure:

Magnetic stirrer and an ultraviolet/visible spectrophotometer.

Solubility was determined by stirring an excess of solute in the solvent with a magnetic stirrer at ambient room temperature for 24 h in sealed flasks that were thermally insulated from the stirrer. The suspension was gravity filtered through Whatman #1 (qualitative) filter paper. The filtrate was then quantitatively diluted with methanol, and the absorbance of the diluted solution recorded at 306 nm.

Source and Purity of Chemicals:

(1) Purity not given, Aldrich Chemical Company, Milwaukee, WI, USA, no purification details were provided.

(2) Purity not given, Fisher Scientific, Orlando, FL, USA, used as received.

Estimated Error:

Temperature: ±1 K.

x_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl 2-hydroxypropanoate; $C_5H_{10}O_3$; [97-64-3]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 194.4 mg/ml, which corresponds to a molar solubility of $c_1 = 1.407$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:

(1) Purity not given, Fisher Scientific Equipment, UK, no purification details were provided.

(2) Purity not given, Purac Biochem, Gorinchem, Netherlands, no purification details were provided.

Estimated Error:

Temperature: Insufficient experimental details to estimate.

c_1: ±0.046.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 1-Methylethyl 2-hydroxypropanoate; $C_6H_{12}O_3$; [617-64-3]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 222.34 mg/ml, which corresponds to a molar solubility of $c_1 = 1.610$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Purac Biochem, Gorinchem, Netherlands, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.29.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Butyl 2-hydroxypropanoate; $C_7H_{14}O_3$; [138-22-7]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 234.1 mg/ml, which corresponds to a molar solubility of $c_1 = 1.695$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Purac Biochem, Gorinchem, Netherlands, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.11.

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) 9(Z)-Octadecenoic acid (Oleic acid); $C_{18}H_{34}O_2$; [112-80-1]	[87]M. Dias, J. Hadgraft, and M. E. Lane, Int. J. Pharm. **336**, 108 (2007).
Variables:	**Prepared by:**
T/K = 305.2	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 121.20 mg/ml, which corresponds to a molar solubility of $c_1 = 0.877$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were equilibrated in a constant-temperature bath with stirring for 48 h. The saturated solution was then centrifuged for 10 min, and an aliquot of the supernatant solution was removed and diluted quantitatively for spectrophotometric analysis. The concentration of the dissolved solute was determined from the measured absorbance.

Source and Purity of Chemicals:
(1) Purity not given, Fisher Scientific Equipment, UK, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Insufficient experimental details to estimate.
c_1: ±0.024.

46.11. 2-Hydroxybenzoic acid solubility data in binary organic solvent mixtures

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethanol; C_2H_6O; [64-17-5] (3) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[152]H. Matsuda, K. Kaburagi, S. Matsumoto, K. Kurihara, K. Tochigi, and K. Tomono, J. Chem. Eng. Data **54**, 480 (2009).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$x_2^{(s)}$[a]	x_2[b]	x_1[c]
0.0000	0.0000	0.1383
0.1613	0.1346	0.1653
0.2991	0.2462	0.1767
0.4201	0.3441	0.1810
0.5262	0.4311	0.1808
0.6277	0.5123	0.1839
0.7134	0.5894	0.1738
0.7947	0.6553	0.1754
0.8701	0.7295	0.1616
0.9389	0.8031	0.1446
1.0000	0.8550	0.1450

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Thermostated constant-temperature water bath and high-performance liquid chromatograph with an uv detector.

Excess solute and solvent were allowed to equilibrate for 24 h in a constant-temperature thermostated water bath. Aliquots of saturated solutions were removed and filtered through a membrane filter of 0.45 μm pore size (Millipore, USA). Concentrations were determined by high-performance liquid chromatography equipped with an uv detector (254 nm detection). Benzene was added to the sample as an internal standard.

Source and Purity of Chemicals:

(1) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.

(2) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.

(3) 99.5%, Wako Pure Chemical Industries, Ltd., Japan, was used without further purification.

Estimated Error:

Temperature: ±0.05 K.

$x_2^{(s)}$: ±0.0001.

x_1: ±6.2% (relative error).

Components:

(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7]

(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

(3) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:

[155]M. A. Peña, A. Reíllo, B. Escalera, and P. Bustamante, Int. J. Pharm. **321**, 155 (2006).

Variables:

T/K = 298.15; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	$v_2^{(s)\,a}$	$x_1^{\,c}$
298	0.00	0.1397
298	0.10	0.1458
298	0.20	0.1579
298	0.30	0.1653
298	0.40	0.1749
298	0.50	0.1830
298	0.60	0.1893
298	0.70	0.1854
298	0.80	0.1658
298	0.90	0.1309
298	1.00	0.1136

[a] $v_2^{(s)}$: initial volume fraction of component 2 in the binary solvent mixture.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.

Binary solvent mixtures were prepared by volume. Excess solute and solvent were allowed to equilibrate in a constant temperature-controlled shaking bath for at least five days. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 302 nm. The authors converted the molar solubilities to mole fractions using the measured densities of the saturated solutions.

Source and Purity of Chemicals:

(1) Purity not given, Sigma-Aldrich, Munich, Germany, was used as received.

(2) UV grade, anhydrous, Panreac, Monplet and Esteban, Barcelona, Spain, was used as received.

(3) UV grade, anhydrous, Panreac, Monplet and Esteban, Barcelona, Spain, was used as received.

Estimated Error:

Temperature: ±0.1 K.

$v_2^{(s)}$: ±0.01.

x_1: ±3% (relative error, most of the experimental values had uncertainties of 3% or less).

Components:

(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7]

(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

(3) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:

[154]M. A. Peña, B. Escalera, A. Reíllo, A. B. Sánchez, and P. Bustamante, J. Pharm. Sci. **98**, 1129 (2009).

Variables:

Temperature; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	$v_2^{(s)\,a}$	$x_1^{\,c}$
293	0.00	0.1348
293	0.10	0.1408
293	0.20	0.1529
293	0.30	0.1602
293	0.40	0.1697
293	0.50	0.1780
293	0.60	0.1844
293	0.70	0.1784
293	0.80	0.1608
293	0.90	0.1259
293	1.00	0.1085
303	0.00	0.1405
303	0.10	0.1550
303	0.20	0.1673
303	0.30	0.1750
303	0.40	0.1859
303	0.50	0.1948
303	0.60	0.1984
303	0.70	0.1950
303	0.80	0.1750
303	0.90	0.1435
303	1.00	0.1219
308	0.00	0.1485
308	0.10	0.1655
308	0.20	0.1747
308	0.30	0.1851
308	0.40	0.1948
308	0.50	0.1980
308	0.60	0.2031
308	0.70	0.2019
308	0.80	0.1807
308	0.90	0.1554
308	1.00	0.1293
313	0.00	0.1605
313	0.10	0.1726
313	0.20	0.1873

T/K	$v_2^{(s)}$ [a]	x_1 [c]
313	0.30	0.1948
313	0.40	0.2019
313	0.50	0.2071
313	0.60	0.2104
313	0.70	0.2100
313	0.80	0.1918
313	0.90	0.1609
313	1.00	0.1329

[a] $v_2^{(s)}$: initial volume fraction of component 2 in the binary solvent mixture.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant temperature-controlled shaking bath and an uv/visible spectrophotometer.
Binary solvent mixtures were prepared by volume. Excess solute and solvent were allowed to equilibrate in a constant temperature-controlled shaking bath for four days at 313 K, and then one day at the lower temperatures. The authors used the same samples for all temperatures. The authors started with 313 K, and once the solution was saturated at the higher temperature they lowered the temperature for the next set of measurements. Aliquots of the saturated solution were removed and filtered (Durapore membrane filter, 0.2 μm pore size). The filtered aliquot was then diluted with ethanol (96% v/v), and the concentration of the dissolved solute determined by spectrophotometric analysis at a wavelength of 302 nm. The authors converted the molar solubilities to mole fractions using the measured densities of the saturated solutions.

Source and Purity of Chemicals:
(1) Purity not given, Sigma-Aldrich, Munich, Germany, was used as received.
(2) UV grade, anhydrous, Panreac, Monplet and Esteban, Barcelona, Spain, was used as received.
(3) UV grade, anhydrous, Panreac, Monplet and Esteban, Barcelona, Spain, was used as received.

Estimated Error:
Temperature: ±0.1 K.
$v_2^{(s)}$: ±0.01.
x_1: ±3% (relative error, most of the experimental values had uncertainties of 3% or less).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Propanone; C_3H_6O; [67-64-1] (3) Benzene; C_6H_6; [71-43-2]	[149]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **39**, 1 (1917).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$w_2^{(s)}$ [a]	s_1 [b]	m_1 [c]
0.00	0.92	0.067
0.10	7.1	0.514
0.20	15.0	1.086
0.40	25.3	1.832
0.60	36.7	2.657
0.80	46.4	3.359
0.90	51.1	3.700
1.00	55.5	4.018

[a] $w_2^{(s)}$: initial mass fraction of component 2 in the binary solvent mixture.
[b] s_1: solubility of the solute given as grams of solute per 100 g of solvent.
[c] m_1: solubility of the solute given as moles of solute per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath.
Binary solvent mixtures were prepared by mass. Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification details were not provided.
(2) Purity not given, Chemical source not given, purification details were not provided.
(3) Purity not given, Chemical source not given, purification details were not provided.

Estimated Error:
Temperature: ±0.1 K.
$w_2^{(s)}$: ±0.01.
m_1: ±10% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6] (3) Benzene; C_6H_6; [71-43-2]	[149]J. W. Marden and M. V. Dover, J. Am. Chem. Soc. **39**, 1 (1917).
Variables:	**Prepared by:**
T/K = 298.15; Solvent Composition	W. E. Acree, Jr.

Experimental Values

$w_2^{(s)}$ [a]	s_1 [b]	m_1 [c]
0.00	0.92	0.067
0.10	3.42	0.248
0.20	6.2	0.449
0.40	12.8	0.927
0.60	16.6	1.202
0.80	22.7	1.643
0.90	24.2	1.752
1.00	38.0	2.751

[a] $w_2^{(s)}$: initial mass fraction of component 2 in the binary solvent mixture.
[b] s_1: solubility of the solute given as grams of solute per 100 g of solvent.
[c] m_1: solubility of the solute given as moles of solute per kilogram of solvent.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature thermostat, analytical balance, and a steam bath. Binary solvent mixtures were prepared by mass. Excess solute and solvent were placed in a bottle with ground glass stopper which was protected by a coating of beeswax and rosin, over which was tied a piece of rubber sheeting. The sealed mixture was shaken in a constant-temperature thermostat for 8–20 h. An aliquot of the saturated solution was withdrawn through a glass wool filter into a weighing pipet from which the solutions were weighed directly into small glass evaporating dishes. The solvent was removed on a steam bath, and the sample further dried in a sulfuric acid desiccator. The solubility was calculated from the mass of the solid residue and the mass of the saturated solution removed for analysis.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, purification details were not provided.
(2) Purity not given, Chemical source not given, purification details were not provided.
(3) Purity not given, Chemical source not given, purification details were not provided.

Estimated Error:
Temperature: ±0.1 K.
$w_2^{(s)}$: ±0.01.
m_1: ±10% (relative error).

Components:	**Original Measurements:**
(1) 2-Hydroxybenzoic acid; $C_7H_6O_3$; [69-72-7] (2) Heptane; C_7H_{16}; [142-82-5] (3) Ethanol; C_2H_6O; [64-17-5]	[163]B. Bouillot, S. Teychené, and B. Biscans, Ind. Eng. Chem. Res. **52**, 9276 (2013).
Variables:	**Prepared by:**
T/K = 293; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	$v_2^{(s)a}$	$x_1{}^c$
293	0.20	0.128
293	0.40	0.116
293	0.60	0.101
293	0.80	0.0679
293	1.00	0.00168

[a] $v_2^{(s)}$: initial volume fraction of component 2 in the binary solvent mixture.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided in the manuscript. The authors simply state that the solubility measurements were carried out using the classical analytical shake flask method.

Source and Purity of Chemicals:
(1) 99.5%, Fisher Scientific, used as received.
(2) 99+%, Analytical Reagent, Fischer Scientific, used as received.
(3) 99+%, Analytical Reagent, Fischer Scientific, used as received.

Estimated Error:
Temperature: Insufficient experimental detail provided in paper to estimate.
$v_2^{(s)}$: ±0.01.
x_1: Insufficient experimental detail provided in paper to estimate.

47. Solubility of 3-Hydroxybenzoic Acid in Organic Solvents

47.1. Critical evaluation of experimental solubility data

There have been several publications[54,56,127,145,147,158,165] reporting the solubility of 3-hydroxybenzoic acid in organic solvents. Hancock *et al.*[54] measured the solubility of 3-hydroxybenzoic acid in cyclohexane and benzene at 303 K based on a gravimetric method. Ongley[56] measured the solubility of 3-hydroxybenzoic acid in benzene, trichloromethane and tetrachloromethane at 298 K. Bergroth[158] reported solubility data for 3-hydroxybenzoic acid dissolved in methanol, ethanol, 1-propanol, propanone, butanone, and 2-pentanone at 293 K. Benzene is the only solvent for which there are two independent experimental data points; however, it is not possible to directly compare the experimental values as the measurements were performed at different temperatures.

Sidgwick and Ewbank[127] measured the solubility of 3-hydroxybenzoic acid in benzene, ethanol, and 1-butanol as a function of temperature. The internal consistency of the benzene dataset was assessed by curve-fitting the measured mole fraction solubility data to the Modified Apelblat model to yield the following mathematical representation:

$$\ln x_1 = -208.672 + \frac{111.81}{T} + 33.861\,\ln T. \qquad (52)$$

The first experimental solubility value of $x_1 = 0.0070$ at 395.7 K was removed from the regression analysis in order to get a better curve-fit. There were too few data points in the ethanol and 1-butanol datasets to perform a meaningful regression analysis. The average absolute deviations between the observed experimental data and back-calculated values based on Eq. (52) of 15.9% is larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0169$ to $x_1 = 0.738$. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 3-hydroxybenzoic acid in organic solvents are in Secs. 47.2–47.9.

47.2. 3-Hydroxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Hexane; C_6H_{14}; [110-54-3]	[145]G. L. Perlovich, T. V. Volkova, and A. Bauer-Brandl, J. Pharm. Sci. **95**, 1448 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9999	0.00000614
298	0.9999	0.00000917
303	0.9999	0.0000112
310	0.9999	0.0000174
315	0.9999	0.0000262

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration, the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) 99%, Merck Chemicals, Darmstadt, Germany, no purification details provided.
(2) Analytical Reagent grade, SDS, Peypin, France, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_2: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.00000973

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±33% (relative error).

47.3. 3-Hydroxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000504

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
395.7	0.993	0.0070
414.2	0.983	0.0169
427.7	0.970	0.0299
435.2	0.938	0.0624
446.2	0.860	0.140
455.7	0.713	0.287
458.7	0.517	0.483
465.7	0.262	0.738

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 474.5 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:

Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 3.198$, which corresponds to a solubility of $c_1 = 0.000634$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.2	0.9999	0.0000571
307.3	0.9999	0.0000797
319.2	0.9999	0.000132
331.2	0.9998	0.000245
337.2	0.9997	0.000335

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported as grams of solute per 100 g of solvent. Numerical values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator. Prior to titration, the solvent was removed by evaporation under reduced pressure.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

47.4. 3-Hydroxybenzoic acid solubility data in esters

Components:	Original Measurements:
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[165] F. L. Nordström and A. C. Rasmuson, Eur. J. Pharm. Sci. **28**, 377 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9604	0.0396
288.2	0.9569	0.0431
293.2	0.9532	0.0468
298.2	0.9493	0.0507
303.2	0.9444	0.0556
308.2	0.9398	0.0602
313.2	0.9342	0.0658
318.2	0.9283	0.0717
323.2	0.9227	0.0773

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for monoclinic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9483	0.0517
288.2	0.9450	0.0550
293.2	0.9409	0.0591
298.2	0.9358	0.0642
303.2	0.9307	0.0693
308.2	0.9248	0.0752
313.2	0.9186	0.0814
318.2	0.9115	0.0885
323.2	0.9042	0.0958

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for the orthorhombic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.

Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:

(1) 99%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8+%, HiperSolv, VWR Scientific, USA, no purification details were provided.

Estimated Error:

Temperature: ±0.01 K.
x_1: ±2% (relative error).

47.5. 3-Hydroxybenzoic acid solubility data in ethers

Components:	Original Measurements:
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[147] J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
T/K = 290	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 9.73 g/100 ml of solution, which corresponds to a molar concentration of 0.704 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: Not given in paper.
c_1: ±10% (relative error, estimated by compiler).

47.6. 3-Hydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	Original Measurements:
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56] P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 2.629$, which corresponds to a solubility of $c_1 = 0.00235$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 4.699$, which corresponds to a solubility of $c_1 = 0.0000200$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

47.7. 3-Hydroxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Methanol; CH_4O; [67-56-1]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables: T/K = 293.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 27.86 g/100 ml of solution, which corresponds to a molar concentration of 2.017 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Methanol; CH_4O; [67-56-1]	[165]F. L. Nordström and A. C. Rasmuson, Eur. J. Pharm. Sci. **28**, 377 (2006).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9153	0.0847
288.2	0.9107	0.0893
293.2	0.9057	0.0943
298.2	0.9002	0.0998
303.2	0.8950	0.1050
308.2	0.8891	0.1109
313.2	0.8823	0.1177
318.2	0.8749	0.1251
323.2	0.8683	0.1317

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for monoclinic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.8%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8%, HiperSolv, VWR Scientific, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Ethanol; C_2H_6O; [64-17-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
338.2	0.821	0.179
405.2	0.654	0.346
442.2	0.402	0.598

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 474.5 K.
(2) 99%, Chemical source not given, distilled over calcium oxide shortly before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Ethanol; C_2H_6O; [64-17-5]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 22.54 g/100 ml of solution, which corresponds to a molar concentration of 1.632 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) 1-Propanol; C_3H_8O; [71-23-8]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 16.34 g/100 ml of solution, which corresponds to a molar concentration of 1.183 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
309.7	0.877	0.123
388.2	0.730	0.270
424.4	0.562	0.438
453.5	0.252	0.748

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 474.5 K.
(2) Purity not given, Chemical source not given, fractionated and distilled several times before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[145]G. L. Perlovich, T. V. Volkova, and A. Bauer-Brandl, J. Pharm. Sci. **95**, 1448 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9163	0.0837
298	0.9056	0.0944
303	0.9007	0.0993
310	0.887	0.113
315	0.878	0.122

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration, the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) 99%, Merck Chemicals, Darmstadt, Germany, no purification details provided.
(2) Analytical Reagent grade, Sigma-Aldrich, Inc., Oslo, Norway, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_2: ±2.5% (relative error).

47.8. 3-Hydroxybenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Propanone; C_3H_6O; [67-64-1]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 20.72 g/100 ml of solution, which corresponds to a molar concentration of 1.500 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Propanone; C_3H_6O; [67-64-1]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables: T/K = 296	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 22.7 g/100 ml of solution, which corresponds to a molar concentration of 1.643 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
c_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Propanone; C_3H_6O; [67-64-1]	[165]F. L. Nordström and A. C. Rasmuson, Eur. J. Pharm. Sci. **28**, 377 (2006).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.8994	0.1006
288.2	0.8942	0.1058
293.2	0.8883	0.1117
298.2	0.8827	0.1173
303.2	0.8759	0.1241
308.2	0.8691	0.1309
313.2	0.8614	0.1386
318.2	0.8549	0.1451
323.2	0.8468	0.1532

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for the monoclinic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.8812	0.1188
288.2	0.8760	0.1240
293.2	0.8702	0.1298
298.2	0.8631	0.1369
303.2	0.8554	0.1446
308.2	0.8473	0.1527
313.2	0.8392	0.1608
318.2	0.8298	0.1702
323.2	0.8185	0.1815

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for the orthorhombic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8+%, HiperSolv, VWR Scientific, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) 2-Butanone; C_4H_8O; [78-93-3]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables: T/K = 293.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 15.69 g/100 ml of solution, which corresponds to a molar concentration of 1.136 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) 2-Pentanone; $C_5H_{10}O$; [107-87-9]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 12.63 g/100 ml of solution, which corresponds to a molar concentration of 0.914 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

47.9. 3-Hydroxybenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[165]F. L. Nordström and A. C. Rasmuson, Eur. J. Pharm. Sci. **28**, 377 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9780	0.0220
288.2	0.9756	0.0244
293.2	0.9727	0.0273
298.2	0.9697	0.0303
303.2	0.9665	0.0335
308.2	0.9624	0.0376
313.2	0.9585	0.0415
318.2	0.9538	0.0462
323.2	0.9488	0.0512

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for the monoclinic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9709	0.0291
288.2	0.9689	0.0311
293.2	0.9659	0.0341
298.2	0.9625	0.0375
303.2	0.9585	0.0415
308.2	0.9541	0.0459
313.2	0.9489	0.0511
318.2	0.9439	0.0561
323.2	0.9386	0.0614

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for the orthorhombic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 96%, Pro Analysis, Merck Chemical Company, Germany, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

Components:	**Original Measurements:**
(1) 3-Hydroxybenzoic acid; $C_7H_6O_3$; [99-06-9] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[165]F. L. Nordström and A. C. Rasmuson, Eur. J. Pharm. Sci. **28**, 377 (2006).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9929	0.0071
288.2	0.9918	0.0082
293.2	0.9904	0.0096
298.2	0.9889	0.0111
303.2	0.9870	0.0130
308.2	0.9846	0.0154
313.2	0.9821	0.0179
318.2	0.9799	0.0201
323.2	0.9766	0.0234

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for the monoclinic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9910	0.0090
288.2	0.9897	0.0103
293.2	0.9881	0.0119
298.2	0.9861	0.0139
303.2	0.9839	0.0161
308.2	0.9811	0.0189
313.2	0.9781	0.0219
318.2	0.9745	0.0255
323.2	0.9706	0.0294

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The authors noted that the solid existed in different polymorphic forms. The solubility data are for the orthorhombic form. Solubilities were reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath for at least 24 h with stirring. The stirring was discontinued and the solid was allowed to settle to the bottom of the container. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8+%, LiChroSolv, VWR Scientific, USA, no purification details were provided.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±2% (relative error).

48. Solubility of 4-Hydroxybenzoic Acid in Organic Solvents

48.1. Critical evaluation of experimental solubility data

There have been several published studies[54,56,77,127,147,166–168] involving the solubility of 4-hydroxybenzoic acid in organic solvent mixtures. Most notably, Martin *et al.*[166] performed solubility measurements at 298 K for 4-hydroxybenzoic acid in two aromatic hydrocarbons (benzene and methylbenzene), in two alkyl alkanoates (ethyl ethanoate and butyl ethanoate) in one dialkyl ether (1,1′-oxybisethane) and one cyclic ether (1,4-dioxane), in two chloroalkanes (trichloromethane and 1,2-dichloroethane), in 13 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-methyl-1-propanol, 1-pentanol, 1-hexanol, 1-octanol, benzenemethanol, 1,2-ethanediol, 1,2-propanediol, and 1,2,3-propanetriol), in one alkanone (propanone) and one aromatic ketone (acetophenone), and in eight miscellaneous organic solvents (ethanoic acid, propanoic acid, dimethyl sulfoxide, pyridine, formamide, *N*-methylformamide, *N*,*N*-dimethylformamide, and *N*,*N*-dimethylacetamide). Gracin and Rasmuson[167] determined the solubility of 4-hydroxybenzoic acid in ethyl ethanoate, methanol, ethanol, 2-propanol, 1-octanol, and propanone at 298 K.

The Abraham solvation parameter model can provide an indication of the quality of experimental solubility data for 4-hydroxybenzoic acid dissolved in a series of organic solvents of varying polarity and hydrogen bonding character. As discussed above, the evaluation will be restricted to those solvents where dimerization is not likely to occur and to solvents where 4-hydroxybenzoic acid does not form a solid solvate. This condition will limit the evaluation to primarily the alkyl alkanoates, dialkyl ethers, and alcohols.

TABLE 38. Comparison between observed and predicted molar solubilities of 4-hydroxybenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{exp}}$
Methanol	0.327	0.225	0.377[a]	0.377[b]
Ethanol	0.329	0.271	0.276[a]	0.292[b]
1-Propanol	0.158	0.159	0.142[a]	
2-Propanol	0.185	0.205	0.208[a]	0.228[b]
1-Butanol	−0.008	−0.003	0.092[a]	
2-Butanol	0.042	0.043		
2-Methyl-1-propanol	−0.004	−0.058	−0.016[a]	
2-Methyl-2-propanol	0.098	0.189		
1-Pentanol	0.061	0.058	0.025[a]	
2-Pentanol	0.101	0.054		
3-Methyl-1-butanol	−0.014	−0.089		
1-Hexanol	−0.038	−0.054	−0.040[a]	
1-Heptanol	−0.214	−0.105		
1-Octanol	−0.202	−0.241	−0.170[a]	−0.141[b]
1-Decanol	−0.209	−0.210		
1,2-Ethanediol	0.219	0.263	0.266[a]	
1,1′-Oxybisethane	−0.468	−0.405	−0.300[a]	
Tetrahydrofuran	0.198	0.174		
1,4-Dioxane	−0.148	−0.186	−0.014[a]	
Methyl ethanoate	−0.486	−0.553		
Ethyl ethanoate	−0.403	−0.411	−0.128[a]	−0.151[b]
Propyl ethanoate	−0.496	−0.520		
Butyl ethanoate	−0.589	−0.629	−0.358[a]	
Propanone	−0.226	−0.230	0.184[a]	0.187[b]

[a]Experimental value is taken from Martin *et al.*[166]

[b]Gracin and Rasmuson.[167]

Numerical values of the solute descriptors for 4-hydroxybenzoic acid are known ($E = 0.930$, $S = 0.900$, $A = 0.810$, $B = 0.570$, $V = 0.9904$, and $L = 4.867$), so that combination of these descriptors with the coefficients listed in Table 1 allows the prediction of $\log_{10} (c_{1,\mathrm{S}}^{\mathrm{sat}} / c_{1,\mathrm{W}}^{\mathrm{sat}})$. The molar solubility of molecular 4-hydroxybenzoic acid in water, $\log_{10} c_{1,\mathrm{W}}^{\mathrm{sat}} = -1.47$ (Ref. 164), is available to convert the predicted $(c_{1,\mathrm{S}}^{\mathrm{sat}} / c_{1,\mathrm{W}}^{\mathrm{sat}})$ solubility ratios to $c_{1,\mathrm{S}}^{\mathrm{sat}}$ values. For carboxylic acid solutes, $c_{1,\mathrm{W}}^{\mathrm{sat}}$ corresponds to the aqueous solubility of the molecular, nonionized form of the solute. A numerical value of $\log_{10} c_{1,\mathrm{G}} = -8.25$ is used for the gas-phase molar concentration of 4-hydroxybenzoic acid.

The predicted molar solubilities of 4-hydroxybenzoic acid in methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-octanol, 2-propanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1,2-ethanediol, 1,1′-oxybisethane, tetrahydrofuran, 1,4-dioxane, ethyl ethanoate, butyl ethanoate, propanone, butanone, and cyclohexanone based on Eqs. (20) and (21) are listed in the second and third columns of Table 38. The numerical values represent outright solubility predictions in that none of the experimental data was used in the determination of the molecular solute descriptors. For comparison purposes, the measured mole fraction solubilities of 4-hydroxybenzoic acid, x_1, given in Secs. 48.2–48.9 were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 4-hydroxybenzoic acid is taken to be $V_{\mathrm{solute}} = 104\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$, which is larger than the value that other researchers have used. Martin *et al.*[166] assumed a molar volume of 4-hydroxybenzoic acid of $V_1 = 94.3\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$. This latter value seems too small compared to the molar volume of benzaldehyde, which is estimated to be $V_1 \approx 101.7\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$, based on a molar mass of 106.12 g mol^{-1} and an experimental density of 1.0436 g cm^{-3} at 298 K. A molar volume on the order of $V_1 \approx 104\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$ would seem more realistic given the molecular structures of 4-hydroxybenzoic acid compared to benzaldehyde. To get an idea of how much error might be introduced in the mole fraction to molarity conversion, the mole fraction solubility of 4-hydroxybenzoic acid in methanol of $x_1 = 0.1142$ (value from Martin *et al.*[166]) is converted into molar solubilities using both $V_1 = 94.3\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$ ($c_1 = 2.439\ \mathrm{mol\,dm}^{-3}$) and $V_1 \approx 104\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$ ($c_1 = 2.383\ \mathrm{mol\,dm}^{-3}$). Results of the computation suggest that any errors resulting from the estimation of 4-hydroxybenzoic acid's hypothetical subcooled liquid molar volume, V_{solute}, or the ideal molar volume approximation will have negligible effect of the calculated c_1 values because 4-hydroxybenzoic acid is not overly soluble in many of the solvents considered. From a mathematical standpoint, the $x_1^{\mathrm{exp}} V_{\mathrm{solute}}$ term contributes very little to the molar volumes of the saturated solutions.

There is a sufficient number of data points for several of the solvents in Secs. 48.2–48.9 to compute a recommended value. The recommended mole fraction solubilities at 298 K are: $x_1 = 0.0719$ for ethyl ethanoate [arithmetic average of $x_1 = 0.0737$,[166] 0.0698,[167] and 0.0722 (Ref. 168)]; $x_1 = 0.114$ for methanol [arithmetic average of $x_1 = 0.1142$,[166] 0.1142,[167] and 0.1141 (Ref. 168)]; and $x_1 = 0.106$ for 1-octanol [arithmetic average of 0.1031,[166] 0.1102,[167] and 0.106,[77] excluding a suspected outlier value of $x_1 = 0.139$ (Ref. 145)].

Nordström and Rasmuson[168] measured the solubility of 4-hydroxybenzoic acid in ethyl ethanoate, methanol, propanone, ethanenitrile, and ethanoic acid at several temperatures between 283 K and 323 K in order to calculate thermodynamic data pertaining to the dissolution process. The authors computed the enthalpy of solution of 4-hydroxybenzoic acid in the five organic solvents through a Van't Hoff treatment of the measured solubility data. The natural logarithms of the mole fraction solubilities were curve-fit to a second degree polynomial in $1/T$

$$\ln x_1 = A + \frac{B}{T} + \frac{C}{T^2}, \tag{53}$$

with the enthalpy of solution calculated as the temperature derivative, i.e., $\Delta H_{\mathrm{soln}} = RT^2(\mathrm{d}\ln x_1/\mathrm{d}T)$. The equation coefficients (A, B, and C), along with the squared correlation coefficients, R^2, are given in Table 39. The authors did note in the discussion the morphologies of crystals obtained by evaporation crystallization from the different solvents, and some of the difficulties encountered in making reproducible solubility measurements. Solubility analyses and FTIR-ATR spectroscopic measurements, in combination with the solubility analyses and microscopic examinations, did suggest indications of an enantiotropic polymorphism in ethanenitrile and ethanoic acid. The transition point was estimated to fall between 298 and 303 K. An acetone solvate was found and

TABLE 39. Parameters of Eq. (53) for describing the solubility of 4-hydroxybenzoic acid in various organic solvents

Solvent	A	B	C	R^2
Ansolvate[a]				
Methanol	5.3439	−3688.6	432010	0.9981
Ethanenitrile	8.1099	−4864.5	351270	0.9993
Ethanoic acid	6.7801	−4499.5	466550	0.9999
Propanone	13.414	−8727.2	124350	0.9985
Ethyl ethanoate	6.0428	−4137.8	462870	0.9999
Solvate[a]				
Acetone solvate	10.286	−5873.3	647790	0.9999

[a]Values of the coefficients and squared correlation coefficients were taken from Nordström and Rasmuson.[168]

shown to be the stable phase up to approximately 323 K. The solubility of the ansolvate could be determined at higher temperature by dissolution up to equilibrium. Both propanone and 4-hydroxybenzoic acid had to be preheated to 323 K in order to inhibit phase conversion into the solvate. The authors were able to measure the solubility of the ansolvate down to 303 K. Indication of the presence of further solvates in ethanenitrile, ethyl ethanoate, and methanol was found but could not be verified.

Qingzhu *et al.*[77] measured the solubility of 4-hydroxybenzoic acid in 1-octanol as a function of temperature using a dynamic method with laser monitoring to observe when dissolution was complete. The calculated curve-fit parameters from the Buchowski λh-model [Eq. (9)] of $\lambda = 0.0248$ and $h = 5861.21$ described the observed solubility data to within a mean relative deviation of 0.2%.

The experimental solubility data for 4-hydroxybenzoic acid in organic solvents are in Secs. 48.2–48.9.

48.2. 4-Hydroxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Hexane; C_6H_{14}; [110-54-3]	[145]G. L. Perlovich, T. V. Volkova, and A. Bauer-Brandl, J. Pharm. Sci. **95**, 1448 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.9999	0.00000205
294	0.9999	0.00000245
298	0.9999	0.00000305
303	0.9999	0.00000376
310	0.9999	0.00000596
315	0.9999	0.00000714

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration, the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) 99%, Merck Chemicals, Darmstadt, Germany, no purification details provided.
(2) Analytical Reagent grade, Sigma-Aldrich Inc., Oslo, Norway, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_2: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000370

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 4.398$, which corresponds to a solubility of $c_1 = 0.0000400$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

48.3. 4-Hydroxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.000038

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000588

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
405.4	0.994	0.0059
430.1	0.983	0.0174
438.5	0.975	0.0248
451.2	0.939	0.0610
464.7	0.869	0.131
468.9	0.721	0.279
472.0	0.527	0.473
479.2	0.266	0.734

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 486.2 K.

(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 3.432$, which corresponds to a solubility of $c_1 = 0.000370 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, solute was either “AnalaR” grade or recrystallized prior to use.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: No information was given.

c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9999	0.0000111
306.2	0.9999	0.0000323
322.2	0.9999	0.0000876
337.2	0.9998	0.000198
353.2	0.9996	0.000373

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported as grams of solute per 100 g of solvent. Numerical values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator. Prior to titration, the solvent was removed by evaporation under reduced pressure.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Toluene; C_7H_8; [108-88-3]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.000027

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Toluene; C_7H_8; [108-88-3]	[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9990	0.00100

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) 99.5%, Kemetyl AB, Sweden, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±60% (relative error, based on standard deviation given in the paper).

48.4. 4-Hydroxybenzoic acid solubility data in esters

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9263	0.0737

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7]
(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

Original Measurements:
[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9302	0.0698

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) Pro Analyse, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1% (relative error).

Components:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7]
(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

Original Measurements:
[168]F. Nordström and A. C. Rasmuson, J. Pharm. Sci. **95**, 748 (2006).

Variables:
Temperature

Prepared by:
W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9389	0.0611
288.2	0.9356	0.0644
293.2	0.9320	0.0680
298.2	0.9278	0.0722
303.2	0.9233	0.0767
308.2	0.9189	0.0811
313.2	0.9135	0.0865
318.2	0.9084	0.0916
323.2	0.9027	0.0973

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility was reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99+%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8%, HiperSolv, VWR Scientific, USA, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±3% (relative error, estimated by compiler).

Components:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7]
(2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]

Original Measurements:
[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9426	0.0574

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Methylethyl tetradecanoate; $C_{17}H_{34}O_2$; [110-27-0]	[61]E. R. Cooper, J. Controlled Release **1**, 153 (1984).
Variables: T/K = 295	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.984	0.016

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Aldrich Chemical Company, Metuchen, NJ, USA, no purification details provided.
(2) Reagent grade, Wickhen Corporation, Huguenot, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

48.5. 4-Hydroxybenzoic acid solubility data in ethers

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9479	0.0521

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables: T/K = 290	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 9.43 g/100 ml of solution, which corresponds to a molar concentration of 0.683 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:

Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, no purification details were provided.

(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.707	0.293

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.

Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.

(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:

Temperature: ±0.02 K.

x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9156	0.0844

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath and ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.

(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:

Temperature: ±0.2 K.

x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.851	0.149

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

48.6. 4-Hydroxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9998	0.00015

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 2.991$, which corresponds to a solubility of $c_1 = 0.00102$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 5.000$, which corresponds to a solubility of $c_1 = 0.0000100$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-60-2]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.00011

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

48.7. 4-Hydroxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Methanol; CH_4O; [67-56-1]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8858	0.1142

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Methanol; CH_4O; [67-56-1]	[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8858	0.1142

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) Pro Analyse, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Methanol; CH_4O; [67-56-1]	[168]F. Nordström and A. C. Rasmuson, J. Pharm. Sci. **95**, 748 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.8987	0.1013
288.2	0.8961	0.1039
293.2	0.8902	0.1098
298.2	0.8859	0.1141
303.2	0.8795	0.1205
308.2	0.8746	0.1254
313.2	0.8693	0.1307
318.2	0.8617	0.1383
323.2	0.8556	0.1444

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility was reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99+%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8%, HiperSolv, VWR Scientific, USA, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Methanol; CH_4O; [67-56-1]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 32.45 g/100 ml of solution, which corresponds to a molar concentration of 2.349 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethanol; C_2H_6O; [64-17-5]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8787	0.1213

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethanol; C_2H_6O; [64-17-5]	[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8739	0.1261

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) 99.5%, Kemetyl AB, Sweden, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethanol; C_2H_6O; [64-17-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
340.2	0.826	0.174
409.7	0.658	0.342
457.2	0.382	0.618

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 486.2 K.
(2) 99%, Chemical source not given, distilled over calcium oxide shortly before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethanol; C_2H_6O; [64-17-5]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 24.36 g/100 ml of solution, which corresponds to a molar concentration of 1.699 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8916	0.1084

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables: T/K = 293.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 19.46 g/100 ml of solution, which corresponds to a molar concentration of 1.409 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 2-Propanol; C_3H_8O; [67-63-0]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8703	0.1297

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 2-Propanol; C_3H_8O; [67-63-0]	[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8639	0.1361

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) Pro Analyse, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8846	0.1154

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
305.7	0.885	0.115
335.2	0.848	0.152
389.3	0.741	0.259
440.2	0.529	0.471
467.0	0.240	0.760

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 486.2 K.
(2) Purity not given, Chemical source not given, fractionated and distilled several times before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9099	0.0901

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8855	0.1145

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8879	0.1121

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8968	0.1032

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8898	0.1102

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) Pro Analyse, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[77]J. Qingzhu, M. Peisheng, Y. Shouzhi, W. Qiang, W. Chang, and L. Guiju, J. Chem. Eng. Data **53**, 1278 (2008).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.65	0.8947	0.1053
299.95	0.8928	0.1072
301.45	0.8911	0.1089
302.85	0.8897	0.1103
304.25	0.8885	0.1115
305.85	0.8869	0.1131
306.95	0.8854	0.1146
308.15	0.8841	0.1159
309.85	0.8828	0.1172
311.25	0.8812	0.1188
313.15	0.8794	0.1206
315.45	0.8776	0.1224
317.25	0.8757	0.1243
318.65	0.8740	0.1260
320.55	0.8721	0.1279
322.25	0.8701	0.1299

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating water bath, analytical balance, laser monitoring system.
Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate of 0.5 K/20 min (0.2 K/20 min or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) <99%, Chemical source not specified, used as received.
(2) <99%, Chemical source not specified, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0005.

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[145]G. L. Perlovich, T. V. Volkova, and A. Bauer-Brandl, J. Pharm. Sci. **95**, 1448 (2006).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
293	0.871	0.129
298	0.861	0.139
303	0.846	0.154
310	0.823	0.177
315	0.814	0.186

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated constant-temperature bath, centrifuge, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in a glass ampoule and allowed to equilibrate in a thermostated temperature bath with mixing (at a speed of 25 rpm) for a minimum of four days. After suitable equilibration the saturated solution was centrifuged, the supernatant liquid collected, quantitatively diluted, and the absorbance recorded using an ultraviolet/visible spectrophotometer. The solubility of the solute was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) 99%, Merck Chemicals, Darmstadt, Germany, no purification details provided.
(2) Analytical Reagent grade, Sigma-Aldrich Inc., Oslo, Norway, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K.
x_2: ±2.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Benzenemethanol; C_7H_8O; [100-51-6]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9216	0.0784

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8868	0.1132

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8692	0.1308

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,2-Propanediol; $C_3H_8O_2$; [57-55-6]	[61]E. R. Cooper, J. Controlled Release **1**, 153 (1984).
Variables: T/K = 295	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.845	0.155

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in terms of mass percent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details provided. Solubility determinations were made by stirring the solvent with excess solute for two days, centrifuging the sample, and analyzing the supernatant.

Source and Purity of Chemicals:
(1) Reagent grade, Aldrich Chemical Company, Metuchen, NJ, USA, no purification details provided.
(2) Reagent grade, J.T. Baker Chemical Company, Phillipsburg, NJ, USA, no purification details provided.

Estimated Error:
Temperature: No information given.
x_1: No information given.

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 1,2,3-Propanetriol (Glycerol); $C_3H_8O_3$; [60-29-7]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9699	0.0301

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

48.8. 4-Hydroxybenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Propanone; C_3H_6O; [67-64-1]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8815	0.1185

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Propanone; C_3H_6O; [67-64-1]	[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8806	0.1194

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) Pro Analyse, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Propanone; C_3H_6O; [67-64-1]	[168]F. Nordström and A. C. Rasmuson, J. Pharm. Sci. **95**, 748 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.2	0.8417	0.1583
308.2	0.8371	0.1629
313.2	0.8299	0.1701
318.2	0.8235	0.1765
323.2	0.8145	0.1855

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility was reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99+%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8%, HiperSolv, VWR Scientific, USA, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Propanone; C_3H_6O; [67-64-1]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 20.55 g/100 ml of solution, which corresponds to a molar concentration of 1.488 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Propanone; C_3H_6O; [67-64-1]	[147]J. Walker and J. K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
T/K = 296	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 22.7 g/100 ml of solution, which corresponds to a molar concentration of 1.643 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Excess solute and solvent were equilibrated with agitation by stirrers driven by a small turbine. At higher temperatures agitation was occasionally by hand. Equilibrium was obtained by both undersaturation at lower temperature and by supersaturation by pre-equilibrating at a higher temperature. The concentration of the dissolved solute was determined by titration with barium hydroxide with Congo Red being the endpoint indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: Not given in paper.
c_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 2-Butanone; C_4H_8O; [78-93-3]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 20.58 g/100 ml of solution, which corresponds to a molar concentration of 1.490 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 2-Pentanone; $C_5H_{10}O$; [107-87-9]	[158]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
T/K = 293.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 17.09 g/100 ml of solution, which corresponds to a molar concentration of 1.237 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined using a gravimetric method. Excess solute and solvent were placed in a solubility vessel. The apparatus was closed tightly with rubber stoppers and allowed to equilibrate in a constant-temperature water bath with stirring. A known aliquot of the saturated solution was removed, filtered, and transferred to an evaporating dish. The solvent was carefully removed over a steam bath. The evaporating dish was then placed in a drying oven, and later removed and weighed. The solubility was calculated from the mass of the solid residue and volume of saturated sample analyzed.

Source and Purity of Chemicals:
(1) 99.5%, Schuchardt Chemicals, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) 4-Methyl-2-pentanone; $C_6H_{12}O$; [108-10-1]	[167]S. Gracin and A. C. Rasmuson, J. Chem. Eng. Data **47**, 1379 (2002).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8999	0.1001

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility data were reported as the grams of solute that dissolved per kilogram of solvent. Mole fraction solubility calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostated water bath, analytical balance, magnetic stirrer, and vacuum drying oven.
Solubility was determined by the gravimetric method. Excess solute and solvent were placed in Erlenmeyer flasks and allowed to equilibrate for 72 h in a thermostatic water bath sitting on a multiple-position magnetic stirrer. The solutions were stirred during the equilibration period. The stirring was then stopped for 4 h to allow the suspended solid to settle to the bottom of the flask. A sample of the clear saturated solution was transferred with a heated syringe into a previously weighed sample vial. The vial containing the saturated solution was then weighed, and the solvent was allowed to evaporate in a vacuum oven at 293 K for approximately one week until a constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of the saturated solution analyzed.

Source and Purity of Chemicals:
(1) 99%, Sigma-Aldrich, Sweden, no purification details were provided.
(2) Pro Analyse, Merck Chemical Company, no purification details were provided.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Acetophenone; C_8H_8O; [98-86-2]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9777	0.0223

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

48.9. 4-Hydroxybenzoic acid solubility data in miscellaneous organic solvents

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6326	0.3674

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Pyridine; C_5H_5N; [110-86-1]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8956	0.1044

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Formamide; CH_3NO; [75-12-7]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9659	0.0341

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) *N*-Methylformamide; C_2H_5NO; [123-39-7]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8975	0.1025

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [68-12-2]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7863	0.2137

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) *N*,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7646	0.2354

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer. Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9556	0.0444

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[168]F. Nordström and A. C. Rasmuson, J. Pharm. Sci. **95**, 748 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9628	0.0372
288.2	0.9599	0.0401
293.2	0.9568	0.0432
298.2	0.9531	0.0469
303.2	0.9494	0.0506
308.2	0.9455	0.0545
313.2	0.9412	0.0588
318.2	0.9363	0.0637
323.2	0.9311	0.0689

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. Solubility was reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.
Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:
(1) 99.7%, Merck Chemical Company, Germany, was used as received.
(2) 96%, Pro Analysi, Merck Chemicals, Darmstadt, Germany, used as received.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Propanoic acid; $C_3H_6O_2$; [79-09-4]	[166]A. Martin, P. L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9653	0.0347

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath and ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in screw-capped vials. The vials were sealed and submerged in a constant-temperature water bath and shaken at 100 cycles/min for 24 h. After the 24 h equilibration period, the vial was removed, wiped dry, and the contents analyzed. The solutions were transferred to a syringe and filtered through a 0.1 μm pore size filter. The solutions were diluted and the absorbances recorded at the maximum absorption wavelength of benzoic acid. The solubility was determined at least six times.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, recrystallized from aqueous ethanol before use.
(2) Spectrophotometric or ACS Reagent grade, Chemical source not specified, redistilled before use.

Estimated Error:
Temperature: ±0.2 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Hydroxybenzoic acid; $C_7H_6O_3$; [99-96-7] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[168]F. Nordström and A. C. Rasmuson, J. Pharm. Sci. **95**, 748 (2006).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.9907	0.00927
288.2	0.9894	0.01057
293.2	0.9878	0.0122
298.2	0.9857	0.0143
303.2	0.9833	0.0167
308.2	0.9815	0.0185
313.2	0.9786	0.0214
318.2	0.9755	0.0245
323.2	0.9721	0.0279

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility was reported as grams of solute per kilogram of solvent. Mole fraction values were calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, magnetic stirrer, analytical balance, and ventilated laboratory hood.

Solubilities were determined by a gravimetric method. Excess solute and solvent were placed in sealed bottles and allowed to equilibrate in a constant-temperature bath. An aliquot of the clear solution was removed by syringe, filtered through a 0.2 μm PTFE filter, and transferred to a preweighed glass vial. The glass vial was then weighed, and the solvent was allowed to evaporate in a ventilated laboratory hood at ambient room temperature. Once the solvent had evaporated, the vial with solid residue was weighed until constant weight was obtained. The solubility was calculated from the mass of the solid residue and mass of sample analyzed.

Source and Purity of Chemicals:

(1) 99+%, Sigma-Aldrich Chemical Company, USA, was used as received.
(2) 99.8+%, LiChroSolv, VWR Scientific, USA, used as received.

Estimated Error:

Temperature: ±0.01 K.
x_1: ±3% (relative error, estimated by compiler).

49. Solubility of 2-Hydroxy-3-methylbenzoic Acid in Organic Solvents

49.1. Critical evaluation of experimental solubility data

There has been only a single study involving the solubility of 2-hydroxy-3-methylbenzoic acid in organic solvents. Sidgwick and Ewbank[127] measured the solubility of 2-hydroxy-3-methylbenzoic acid in both heptane and benzene at elevated temperatures. The observed mole fraction solubilities were curve-fit to Eq. (8) to yield the following mathematical representations:

$$\ln x_1 = -140.489 - \frac{2.700}{T} + 23.144 \ln T, \qquad (54)$$

$$\ln x_1 = -91.627 - \frac{1.853}{T} + 15.108 \ln T, \qquad (55)$$

for heptane and benzene, respectively. The experimental data point at 392.2 K had to be excluded from the regression analysis for heptane in order to get a reasonable mathematical correlation. The mean absolute deviations between experimental and calculated values are on the order of 14.5% [Eq. (54)] and 7.6% [Eq. (55)], which are larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0114$ to $x_1 = 0.8275$ for heptane and $x_1 = 0.0094$ to $x_1 = 0.8127$ for benzene. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 2-hydroxy-3-methylbenzoic acid in organic solvents are in Secs. 49.2 and 49.3.

49.2. 2-Hydroxy-3-methylbenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2-Hydroxy-3-methylbenzoic acid; $C_8H_8O_3$; [83-40-9] (2) Heptane; C_7H_{16}; [142-82-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
354.2	0.9886	0.0114
374.2	0.9705	0.0295
392.2	0.9382	0.0618
406.1	0.8360	0.1640
414.1	0.6485	0.3515
415.1	0.6074	0.3926
419.8	0.4178	0.5822
427.5	0.1727	0.8275

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 440.2 K.
(2) Purity not given, sample isolated from the resin of *Pinus sabiniana*, purified by treatment with sulfuric acid and nitric acid, and then distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

49.3. 2-Hydroxy-3-methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Hydroxy-3-methylbenzoic acid; $C_8H_8O_3$; [83-40-9] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
318.4	0.9906	0.0094
335.6	0.9750	0.0250
352.3	0.9526	0.0474
380.4	0.8342	0.1658
396.2	0.6899	0.3101
411.5	0.4808	0.5192
428.6	0.1873	0.8127

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 440.2 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

50. Solubility of 2-Hydroxy-4-methylbenzoic Acid in Organic Solvents

50.1. Critical evaluation of experimental solubility data

There has been only a single study involving the solubility of 2-hydroxy-4-methylbenzoic acid in organic solvents. Sidgwick and Ewbank[127] measured the solubility of 2-hydroxy-4-methylbenzoic acid in both heptane and benzene at elevated temperatures. The observed mole fraction solubilities were curve-fit to Eq. (8) to yield the following mathematical representations:

$$\ln x_1 = -146.021 - \frac{2.939}{T} + 23.876 \ln T, \qquad (56)$$

$$\ln x_1 = -89.757 - \frac{1.876}{T} + 14.728 \ln T, \qquad (57)$$

for heptane and benzene, respectively. The mean absolute deviations between experimental and calculated values are on the order of 19.9% [Eq. (56)] and 7.1% [Eq. (57)], which are larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0127$ to $x_1 = 0.6953$ for heptane and $x_1 = 0.0095$ to $x_1 = 0.8351$ for benzene. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 2-hydroxy-4-methylbenzoic acid in organic solvents are in Secs. 50.2 and 50.3.

50.2. 2-Hydroxy-4-methylbenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2-Hydroxy-4-methylbenzoic acid; $C_8H_8O_3$; [50-85-1] (2) Heptane; C_7H_{16}; [142-82-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
373.8	0.9873	0.0127
389.9	0.9726	0.0274
408.8	0.9379	0.0621
420.3	0.8693	0.1307
429.8	0.7466	0.2534
435.4	0.5172	0.4828
441.9	0.3047	0.6953

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 451.0 K.
(2) Purity not given, sample isolated from the resin of *Pinus sabiniana*, purified by treatment with sulfuric acid and nitric acid, and then distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

50.3. 2-Hydroxy-4-methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Hydroxy-4-methylbenzoic acid; $C_8H_8O_3$; [50-85-1] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
322.0	0.9905	0.0095
344.9	0.9764	0.0236
363.4	0.9523	0.0477
390.8	0.8384	0.1616
408.3	0.6767	0.3233
423.5	0.4594	0.5406
440.8	0.1649	0.8351

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 451.0 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

51. Solubility of 2-Hydroxy-5-methylbenzoic Acid in Organic Solvents

51.1. Critical evaluation of experimental solubility data

There has been only a single study involving the solubility of 2-hydroxy-5-methylbenzoic acid in organic solvents. Sidgwick and Ewbank[127] measured the solubility of 2-hydroxy-5-methylbenzoic acid in both heptane and benzene at elevated temperatures. The observed mole fraction solubilities were curve-fit to Eq. (8) to yield the following mathematical representations:

$$\ln x_1 = -152.882 - \frac{3.209}{T} + 25.256\ \ln T, \qquad (58)$$

$$\ln x_1 = -89.710 - \frac{1.955}{T} + 14.876 \ln T, \qquad (59)$$

for heptane and benzene, respectively. The mean absolute deviations between experimental and calculated values are on the order of 25.2% [Eq. (58)] and 7.1% [Eq. (59)], which are larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0110$ to $x_1 = 0.8414$ for heptane and $x_1 = 0.0083$ to $x_1 = 0.8262$ for benzene. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 2-hydroxy-5-methylbenzoic acid in organic solvents are in Secs. 51.2 and 51.3.

51.2. 2-Hydroxy-5-methylbenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2-Hydroxy-5-methylbenzoic acid; $C_8H_8O_3$; [89-56-5] (2) Heptane; C_7H_{16}; [142-82-5]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
352.2	0.9890	0.0110
370.3	0.9721	0.0279
389.4	0.9352	0.0648
404.3	0.7936	0.2064
408.7	0.6181	0.3819
411.9	0.4195	0.5805
419.1	0.1586	0.8414

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 425.7 K.
(2) Purity not given, sample isolated from the resin of *Pinus sabiniana*, purified by treatment with sulfuric acid and nitric acid, and then distilled before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

51.3. 2-Hydroxy-5-methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Hydroxy-5-methylbenzoic acid; $C_8H_8O_3$; [89-56-5] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.2	0.9917	0.0083
322.0	0.9775	0.0225
341.2	0.9482	0.0518
366.5	0.8341	0.1659
383.8	0.6648	0.3352
397.9	0.4756	0.5244
415.2	0.1738	0.8262

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 425.7 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

52. Solubility of 3-Hydroxy-4-methylbenzoic Acid in Organic Solvents

52.1. Critical evaluation of experimental solubility data

There has been only a single study involving the solubility of 3-hydroxy-4-methylbenzoic acid in organic solvents. Sidgwick and Ewbank[127] measured the solubility of 3-hydroxy-4-methylbenzoic acid in benzene at elevated temperatures. The observed mole fraction solubilities were curve-fit to Eq. (8) to yield the following correlation:

$$\ln x_1 = -178.244 - \frac{3.1001}{T} + 28.896 \ln T. \qquad (60)$$

The mean absolute deviation between experimental and calculated values is on the order of 14.1%, which is larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0102$ to

$x_1 = 0.8369$. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 3-hydroxy-4-methylbenzoic acid in organic solvents are in Sec. 52.2.

52.2. 3-Hydroxy-4-methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-Hydroxy-4-methylbenzoic acid; $C_8H_8O_3$; [586-30-1] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
404.8	0.9898	0.0102
420.6	0.9768	0.0232
433.7	0.9520	0.0480
449.7	0.8353	0.1647
456.9	0.6828	0.3172
465.2	0.4470	0.5530
475.7	0.1631	0.8369

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 481.7 K.

(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. The sample was further purified by freezing several times.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

53. Solubility of 4-Hydroxy-3-methoxybenzoic Acid in Organic Solvents

53.1. Critical evaluation of experimental solubility data

There has been only a single study involving the solubility of 4-hydroxy-3-methoxybenzoic acid (commonly referred to as vanillic acid) in organic solvents. Manic *et al.*[169] measured the solubility of 4-hydroxy-3-methoxybenzoic acid in ethyl 2-hydroxypropanoate at five temperatures between 296 K and 333 K. The observed mole fraction solubilities were curve-fit to Eq. (8) to yield the following correlation:

$$\ln x_1 = -37.631 + \frac{114.97}{T} + 5.916 \ln T. \qquad (61)$$

The mean absolute deviation between experimental and calculated values is on the order of 0.9%, indicating that the experimental data are internally consistent.

The experimental solubility data for 4-hydroxy-3-methoxybenzoic acid in ethyl 2-hydroxypropanoate are in Sec. 53.2.

53.2. 4-Hydroxy-3-methoxybenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Hydroxy-3-methoxybenzoic acid; $C_8H_8O_4$; [121-34-6] (2) Ethyl 2-hydroxypropanoate, $C_5H_{10}O_3$; [687-47-8]	[169]M. S. Manic, D. Villanueva, T. Fornari, A. J. Queimada, E. A. Macedo, and V. Najdanovic-Visak, J. Chem. Thermodyn. **48**, 93 (2012).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.2	0.9721	0.0279
303.1	0.9679	0.0321
312.7	0.9621	0.0379
323.0	0.9556	0.0444
333.3	0.9455	0.0545

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature water bath, stirring plate, and analytical balance. Solubilities were determined using a gravimetric method. Excess solute and solvent were placed in a glass vessel with stirrer. The vessel was placed in a constant-temperature water bath and allowed to equilibrate with stirring for 48 h. After equilibrium had been attained, the stirring was discontinued and the sample was allowed to set for more than 48 h. Samples of the clear saturated solution were removed by micropipette, transferred to a weighed empty vial, and the mass of the vial plus sample were recorded. The sample was placed in a vacuum oven, and the solvent was evaporated at 338 K. Once the solvent had completely evaporated, the mass of the vial and solid residue was determined. The solubility was calculated from the mass of the solid residue and mass of the saturated sample analyzed.

Source and Purity of Chemicals:

(1) 97+%, Fluka Chemical Company, used as received.
(2) 98%, Sigma-Aldrich Chemical Company, dried in a vacuum oven at room temperature for several days prior to use.

Estimated Error:

Temperature: ±0.1 K.
x_1: ±0.0007.

54. Solubility of 4-Hydroxy-3-methylbenzoic Acid in Organic Solvents

54.1. Critical evaluation of experimental solubility data

There has been only a single study involving the solubility of 4-hydroxy-3-methylbenzoic acid in organic solvents. Sidgwick and Ewbank[127] measured the solubility of 4-hydroxy-3-methylbenzoic acid in benzene at elevated temperatures. The observed mole fraction solubilities were curve-fit to Eq. (8) to yield the following correlation:

$$\ln x_1 = -217.192 - \frac{4.4130}{T} + 35.778\ \ln T. \qquad (62)$$

The experimental mole fraction solubility at 439 K had to be excluded in order to obtain a reasonable mathematical correlation. The mean absolute deviation between experimental and calculated values is on the order of 8.3%, which is larger than desired. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to uncertainties in estimating the amount of solvent that remained in the liquid phase, and the large range covered by the experimental values, $x_1 = 0.0131$ to $x_1 = 0.5406$. The derived equation should not be used to predict 4-hydroxy-3-methylbenzoic acid solubilities at temperatures greater than 426 K, as the calculated x_1 values will exceed unity. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 4-hydroxy-3-methylbenzoic acid in benzene are in Sec. 54.2.

54.2. 4-Hydroxy-3-methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Hydroxy-3-methylbenzoic acid; $C_8H_8O_3$; [499-76-3] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
382.7	0.9869	0.0131
389.9	0.9772	0.0228
399.4	0.9503	0.0497
412.7	0.8353	0.1647
418.2	0.6599	0.3401
426.0	0.4594	0.5406
439.2	0.1808	0.8192

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 445.6 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:

Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

55. Solubility of 4-Iodobenzoic Acid in Organic Solvents

55.1. Critical evaluation of experimental solubility data

There has been only one published paper[83] reporting the solubility of 4-iodobenzoic acid in organic solvents. Chantooni and Kolthoff[83] determined the solubility of 4-iodobenzoic acid in methanol, ethanenitrile, dimethyl sulfoxide, and N,N-dimethylformamide at 298 K. It is not possible to perform a critical evaluation of the experimental data as the authors performed measurements at only a single temperature, and there are no independent experimental 4-iodobenzoic acid solubility data in any of the four organic solvents.

The experimental solubility data for 4-iodobenzoic acid in organic solvents are given in Secs. 55.2 and 55.3.

55.2. 4-Iodobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Iodobenzoic acid; $C_7H_5IO_2$; [619-58-9] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.068 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was dehydrated and then distilled over sulfanilic acid to remove alkaline impurities.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

55.3. 4-Iodobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Iodobenzoic acid; $C_7H_5IO_2$; [619-58-9] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.0098 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Iodobenzoic acid; $C_7H_5IO_2$; [619-58-9] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.14 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was shaken with activated alumina and then distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Iodobenzoic acid; $C_7H_5IO_2$; [619-58-9] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.72 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:

Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not given, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.

(2) Purity not given, Chemical source not given, was shaken first with phosphorous pentoxide and then with potassium hydroxide pellets. Solvent was distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K (estimated by compiler).

c_1: ±2% (relative error, estimated by compiler).

56. Solubility of 2-Methoxybenzoic Acid in Organic Solvents

56.1. Critical evaluation of experimental solubility data

There have been four published studies[9,56,72,130] investigating the solubility behavior of 2-methoxybenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Hoover *et al.*[9] measured the solubility of 2-methoxybenzoic acid in 18 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in four alkyl alkanoates (methyl ethanoate, ethyl ethanoate, butyl ethanoate, and pentyl ethanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 2-methoxybenzoic acid. The authors were able to assemble a total of 47 $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 2-methoxybenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -1.554$.[56,72] The McGowan volume of 2-methoxybenzoic acid, $V = 1.1313$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.899$. This left four solute descriptors (S, A, B, and L) still to be determined. The 47 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 1.410$, $A = 0.450$, $B = 0.620$, and $L = 5.636$, that best described the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -8.354$ for the gas-phase solute concentration that made the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (SR or P) and $\log_{10}$ (GSR or K) values to within an average standard deviation of 0.146 and 0.146 $\log_{10}$ units, respectively.

After the 2-methoxybenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, methyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 2-methoxybenzoic acid solubility data. Table 40 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 2-methoxybenzoic acid, x_1, determined by Hoover *et al.*[9] were converted into molar solubilities by dividing x_1 by the

TABLE 40. Comparison between observed and calculated molar solubilities of 2-methoxybenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Methanol	0.267	0.081	0.104
Ethanol	0.074	−0.087	−0.064
1-Propanol	−0.120	−0.217	−0.218
2-Propanol	−0.392	−0.252	−0.235
1-Butanol	−0.247	−0.308	−0.303
2-Butanol	−0.299	−0.257	−0.266
2-Methyl-1-propanol	−0.392	−0.332	−0.336
2-Methyl-2-propanol	−0.286	−0.260	−0.243
1-Pentanol	−0.327	−0.375	−0.379
2-Pentanol	−0.411	−0.383	−0.373
3-Methyl-1-butanol	−0.402	−0.415	−0.401
1-Hexanol	−0.430	−0.407	−0.403
1-Heptanol	−0.471	−0.467	−0.449
1-Octanol	−0.518	−0.485	−0.545
1-Decanol	−0.658	−0.640	−0.626
1,1′-Oxybisethane	−0.638	−0.455	−0.354
Tetrahydrofuran	0.299	0.316	0.309
1,4-Dioxane	0.197	0.240	0.235
Methyl ethanoate	−0.054	0.007	−0.040
Ethyl ethanoate	−0.187	−0.184	−0.169
Butyl ethanoate	−0.447	−0.323	−0.313

ideal molar volume of the saturated solution (i.e., $c_1^{\text{sat}} = x_1/[x_1 V_1 + (1 - x_1)\, V_{\text{solvent}}]$). The molar volume of the hypothetical subcooled liquid 2-methoxybenzoic acid is $V_{\text{solute}} = 124.1\ \text{cm}^3\ \text{mol}^{-1}$. Examination of the numerical entries in Table 40 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Ongley[56] measured the solubility of 2-methoxybenzoic acid in cyclohexane, benzene, trichloromethane, and tetrachloromethane at 298.15 K. Abraham model predictions would not be applicable to these solvents because 2-methoxybenzoic acid would likely dimerize to an appreciable extent. In such cases, the measured solubility would represent the sum of both the monomeric and dimeric forms of the solute. The solute descriptors that have been calculated for 2-methoxybenzoic acid pertain only to the monomeric form. Thuaire[72] reported a mole fraction solubility for 2-methoxybenzoic acid in ethanol of $x_1 = 0.0758$, which differs by less than 1% from the value of $x_1 = 0.0765$ determined by Hoover *et al.*[9]

The experimental solubility data for 2-methoxybenzoic acid in organic solvents are in Secs. 56.2–56.9.

56.2. 2-Methoxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.241$, which corresponds to a solubility of $c_1 = 0.0574\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either “AnalaR” grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

56.3. 2-Methoxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.674$, which corresponds to a solubility of $c_1 = 0.212\ \text{mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either “AnalaR” grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

56.4. 2-Methoxybenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9267	0.0733

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9345	0.0655

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9555	0.0445

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9621	0.0379

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

56.5. 2-Methoxybenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9757	0.0243

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9916	0.00838

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9940	0.00603

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8226	0.1774

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8559	0.1441

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

56.6. 2-Methoxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = -0.225$, which corresponds to a solubility of $c_1 = 1.679$ mol dm$^{-3.}$

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.605$, which corresponds to a solubility of $c_1 = 0.0248$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

56.7. 2-Methoxybenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Methanol; CH_4O; [67-56-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9089	0.0911

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Ethanol; C_2H_6O; [64-17-5]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9235	0.0765

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.780 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.07579$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Propanol; C_3H_8O; [71-23-8]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9405	0.0595

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Propanol; C_3H_8O; [67-63-0]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9537	0.0463

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9466	0.0534

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9526	0.0474

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9617	0.0383

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9502	0.0498

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9481	0.0519

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9573	0.0427

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9573	0.0427

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9600	0.0400

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9533	0.0467

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9562	0.0438

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9591	0.0409

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9522	0.0478

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9523	0.0477

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9584	0.0416

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

56.8. 2-Methoxybenzoic acid solubility data in alkoxyalcohols

Components:	Original Measurements:
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [111-80-5]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8807	0.1193

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8948	0.1052

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9150	0.0850

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8699	0.1301

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8908	0.1092

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) 1-Methyl-2-*tert*-butoxyethanol; $C_7H_{16}O_2$; [57018-52-7]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9236	0.0764

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

56.9. 2-Methoxybenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 2-Methoxybenzoic acid; $C_8H_8O_3$; [579-75-9] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9105	0.0895

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 295 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

57. Solubility of 3-Methoxybenzoic Acid in Organic Solvents

57.1. Critical evaluation of experimental solubility data

There have been four published studies[54,56,63,72] investigating the solubility behavior of 3-methoxybenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Thuaire[72] reported a mole fraction solubility for 3-methoxybenzoic acid dissolved in ethanol. Hancock *et al.*[54,63] measured the solubility of 3-methoxybenzoic acid in cyclohexane, benzene, tetrahydrofuran, and 1,4-dioxane at 303 K based on a gravimetric method. Ongley[56] measured the solubility of 3-methoxybenzoic acid in cyclohexane, benzene, trichloromethane, and tetrachloromethane at 298 K. It is not possible to directly compare the two sets of solubility data as the measurements were performed at different temperatures.

The experimental solubility data for 3-methoxybenzoic acid in organic solvents are in Secs. 57.2–57.6.

57.2. 3-Methoxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9951	0.00493

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.851$, which corresponds to a solubility of $c_1 = 0.0141 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

57.3. 3-Methoxybenzoic acid solubility data in aromatic hydrocarbons

Components:	Original Measurements:
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9558	0.0442

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

Components:	Original Measurements:
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Benzene; C_6H_6; [71-43-2]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.398$, which corresponds to a solubility of $c_1 = 0.400 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

57.4. 3-Methoxybenzoic acid solubility data in ethers

Components:	Original Measurements:
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.691	0.309

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.754	0.246

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

57.5. 3-Methoxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = -0.049$, which corresponds to a solubility of $c_1 = 1.119 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Tetrachloromethane; CCl_4; [56-23-5]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 0.737$, which corresponds to a solubility of $c_1 = 0.183 \text{ mol dm}^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

57.6. 3-Methoxybenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Methoxybenzoic acid; $C_8H_8O_3$; [586-38-9] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 4.216 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1626$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

58. Solubility of 4-Methoxybenzoic Acid in Organic Solvents

58.1. Critical evaluation of experimental solubility data

There have been several published studies[9,54,56,72,130] investigating the solubility behavior of 4-methoxybenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Hoover *et al.*[9] measured the solubility of 4-methoxybenzoic acid in 14 alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 3-methyl-1-butanol, 1-hexanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in three alkanoates (ethyl ethanoate, butyl ethanoate, and pentyl ethanoate) at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 4-methoxybenzoic acid. The authors were able to assemble a total of 44 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 4-methoxybenzoic acid is $\log_{10} c_{1,W} = -2.800$.[72,170] The McGowan volume of 4-methoxybenzoic acid, $V = 1.1313$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.899$. This left four solute descriptors (S, A, B, and L) still to be determined. The 44 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 1.250$, $A = 0.620$, $B = 0.520$, and $L = 5.741$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,G}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,G} = -9.500$ for the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.119 and 0.110 $\log_{10}$ units, respectively.

After the 4-methoxybenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 4-methoxybenzoic acid solubility data. Table 41 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 4-methoxybenzoic acid, x_1, determined by Hoover *et al.*[9] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\text{sat}} = x_1/[x_1V_1 + (1 - x_1)V_{\text{solvent}}]$). The molar volume of the hypothetical subcooled liquid 4-methoxybenzoic acid is $V_{\text{solute}} = 124.1\ \text{cm}^3\ \text{mol}^{-1}$. Examination of the

TABLE 41. Comparison between observed and calculated molar solubilities of 4-methoxybenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\text{exp}}$	$\log_{10} c_1^{\text{calc}}$; Eq. (20)	$\log_{10} c_1^{\text{calc}}$; Eq. (21)
Ethanol	−0.702	−0.753	−0.717
1-Propanol	−0.875	−0.879	−0.839
2-Propanol	−0.864	−0.879	−0.822
1-Butanol	−0.929	−0.987	−0.937
2-Butanol	−0.898	−0.932	−0.905
2-Methyl-1-propanol	−1.100	−1.039	−1.015
2-Methyl-2-propanol	−0.783	−0.889	−0.810
1-Pentanol	−0.984	−1.014	−0.970
2-Pentanol	−0.977	−1.007	−0.958
3-Methyl-1-butanol	−1.079	−1.065	−1.020
1-Hexanol	−1.022	−1.059	−1.020
1-Heptanol	−1.060	−1.109	−1.054
1-Octanol	−1.093	−1.145	−1.161
1-Decanol	−1.174	−1.256	−1.198
1,1′-Oxybisethane	−1.043	−1.157	−1.044
Tetrahydrofuran	−0.162	−0.409	−0.378
1,4-Dioxane	−0.401	−0.619	−0.582
Ethyl ethanoate	−0.879	−0.987	−0.938
Butyl ethanoate	−1.086	−1.139	−1.107

numerical entries in Table 41 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Ongley[56] measured the solubility of 4-methoxybenzoic acid in cyclohexane, benzene, trichloromethane, and tetrachloromethane at 298.15 K. Abraham model predictions would not be applicable to these solvents because 4-methoxybenzoic acid would likely dimerize to an appreciable extent. In such cases, the measured solubility would represent the sum of both the monomeric and dimeric forms of the solute. The solute descriptors that have been calculated for 4-methoxybenzoic acid pertain only to the monomeric form. Thuaire[72] reported a mole fraction solubility for 4-methoxybenzoic acid in ethanol of $x_1 = 0.01242$, which differs by less than 6% from the value of $x_1 = 0.01185$ determined by Hoover *et al.*[9] Differences in chemical purities and experimental methodologies can lead to differences of a few percent between values determined by two different research groups.

The experimental solubility data for 4-methoxybenzoic acid in organic solvents are in Secs. 58.2–58.8.

58.2. 4-Methoxybenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000640

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

58.3. 4-Methoxybenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9983	0.00166

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Benzene; C_6H_6; [71-43-2]	[56] P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.714$, which corresponds to a solubility of $c_1 = 0.0193$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either "AnalaR" grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

58.4. 4-Methoxybenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[9] K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2 [a]	x_1 [b]
0.9869	0.01308

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-864]	[9] K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2 [a]	x_1 [b]
0.9891	0.01087

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9905	0.00949

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

58.5. 4-Methoxybenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9905	0.00952

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9962	0.00377

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9972	0.00275

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9419	0.05811

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.934	0.066

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9652	0.03476

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.959	0.041

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

58.6. 4-Methoxybenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[56]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $-\log_{10} c_1 = 1.130$, which corresponds to a solubility of $c_1 = 0.0741\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Excess solute and solvent were placed in tubes, which were rotated for at least 8 h at 298 K. The solutions were then removed, concentrated if necessary, and titrated with standard alkali using a mixed (bromothymol blue + neutral red) indicator.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, solute was either “AnalaR” grade or recrystallized prior to use.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: No information was given.
c_1: ±4% (relative error, estimated by compiler).

58.7. 4-Methoxybenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Ethanol; C_2H_6O; [64-17-5]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9881	0.01185

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.273 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.01242$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1-Propanol; C_3H_8O; [71-23-8]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9899	0.01008

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Propanol; C_3H_8O; [67-63-0]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9894	0.01060

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9891	0.01088

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9882	0.01175

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9926	0.00740

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9844	0.01561

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9887	0.01130

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9884	0.01156

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9908	0.00916

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9881	0.01190

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9877	0.01234

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9872	0.01275

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[9]K. R. Hoover, D. M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **82**, 1353 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9872	0.01278

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

58.8. 4-Methoxybenzoic acid solubility data in alkoxyalcohols

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9588	0.0412

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9667	0.0333

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9639	0.0361

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4]
(2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]

Original Measurements:
[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9616	0.0384

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4]
(2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]

Original Measurements:
[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9629	0.0371

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Methoxybenzoic acid; $C_8H_8O_3$; [100-09-4]
(2) 1-Methyl-2-*tert*-butoxyethanol; $C_7H_{16}O_2$; [57018-52-7]

Original Measurements:
[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9727	0.0273

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 273 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

59. Solubility of 2-Methylbenzoic Acid in Organic Solvents

59.1. Critical evaluation of experimental solubility data

There have been several published studies[72,77,171–174] investigating the solubility behavior of 2-methylbenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Coaxum *et al.*[171] measured the solubility of 2-methylbenzoic acid in 16 alcohols (ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 1-hexanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in four alkanoates (methyl ethanoate, ethyl ethanoate, butyl ethanoate, and pentyl ethanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 2-methylbenzoic acid. The authors were able to assemble a total of 47 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 2-methylbenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -2.06$.[131,175] The McGowan volume of 2-methylbenzoic acid, $V = 1.0726$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.730$. This left four solute descriptors (*S*, *A*, *B*, and *L*) still to be determined. The 47 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 0.840$, $A = 0.420$, $B = 0.440$, and $L = 4.6770$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -6.360$ for the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.080 and 0.067 $\log_{10}$ units, respectively.

After the 2-methylbenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, methyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 2-methylbenzoic acid solubility data. Table 42 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 2-methylbenzoic acid, x_1, determined by Coaxum *et al.*[171] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 2-methylbenzoic acid is $V_{\mathrm{solute}} = 121.8$ cm^3 mol^{-1}. Examination of the numerical entries in Table 42 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

TABLE 42. Comparison between observed and calculated molar solubilities of 2-methylbenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp,a}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Ethanol	0.325	0.238	0.333
1-Propanol	0.248	0.232	0.242
2-Propanol	0.282	0.221	0.248
1-Butanol	0.205	0.168	0.178
2-Butanol	0.242	0.203	0.208
2-Methyl-1-propanol	0.106	0.152	0.143
2-Methyl-2-propanol	0.329	0.229	0.278
1-Pentanol	0.172	0.181	0.188
2-Pentanol	0.220	0.214	0.200
3-Methyl-1-butanol	0.121	0.169	0.132
1-Hexanol	0.137	0.140	0.149
1-Heptanol	0.103	0.093	0.119
1-Octanol	0.063	0.037	0.021
1-Decanol	0.016	−0.003	0.025
1,1′-Oxybisethane	0.203	0.101	0.172
Tetrahydrofuran	0.456	0.608	0.609
1,4-Dioxane	0.427	0.336	0.338
Methyl ethanoate	0.185	0.162	0.117
Ethyl ethanoate	0.170	0.162	0.169
Butyl ethanoate	0.063	0.067	0.066

[a] Experimental solubility data were taken from Coaxum *et al.*[171]

There are three close independent experimental values in Sec. 59.7 for the solubility of 2-methylbenzoic acid in ethanol. The recommended solubility in ethanol is $x_1 = 0.143$, which is calculated as the arithmetic average of the values of $x_1 = 0.1401$,[171] 0.1460,[72] and 0.142.[173]

Two research groups have studied the solubility behavior of 2-methylbenzoic acid as a function of temperature. Domańska[172,173] determined the solubility of 2-methylbenzoic acid in hexane, heptane, cyclohexane, benzene, 1,2-dimethylbenzene, tetrachloromethane, diiodomethane, chlorobenzene, 1,2-dichlorobenzene, bromobenzene, ethanol, 2-propanol, and nitrobenzene at several temperatures from about 295–345 K based on a dynamic solubility method. The internal consistency of the 13 datasets can be assessed by curve-fitting the measured mole fraction solubilities to Buchowski λh Model [see Eq. (9)]. Table 43 tabulates the equation coefficients (*h* and λ) calculated by the author, along with the corresponding mean standard temperature deviations, σ_T,

$$\sigma_{\mathrm{T}} = \sqrt{\frac{\sum (T_i^{\mathrm{calc}} - T_i^{\mathrm{exp}})^2}{n-1}}, \tag{63}$$

that describe the goodness-of-fit. The summation in Eq. (63) extends over the number of experimental data points, *n*.

TABLE 43. Parameters of the Buchowski λh model for describing the solubility of 2-methylbenzoic acid in various organic solvents[a]

Solvent	T/K	h	λ	σ_T (K)
Hexane	298–332	19550	0.55	0.36
Heptane	292–341	9370	0.52	0.83
Cyclohexane	295–338	5700	1.02	0.87
Benzene	294–345	5200	1.62	0.57
1,3-Dimethylbenzene	297–340	5120	1.61	0.36
Tetrachloromethane	296–336	5270	1.72	0.17
Diiodomethane	294–345	9040	0.83	1.27
Chlorobenzene	299–354	3210	2.44	0.38
1,2-Dichlorobenzene	296–335	4710	1.59	0.33
Bromobenzene	298–352	4850	1.52	0.39
Ethanol	291–337	3450	0.62	0.25
2-Propanol	293–345	3090	0.68	0.42
Nitrobenzene	298–338	5280	1.55	0.22

[a] Values of the coefficients and the mean standard temperature deviations were taken from Domańska.[172]

Qingzhu *et al.*[77] measured the solubility of 2-methylbenzoic acid in 1-octanol from 297 to 322 K employing a laser monitoring method that determined the temperature at which the solid solute was completely dissolved. The authors curve-fit the mole fraction solubilities to Eq. (8) (with $C = 0$). The derived mathematical expression

$$\ln x_1 = 5.432 - \frac{2127}{T} \tag{64}$$

described the experimental x_1 values to within an average absolute relative deviation of 0.8%.

The experimental solubility data for 2-methylbenzoic acid in organic solvents are in Secs. 59.2–59.9.

59.2. 2-Methylbenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Hexane; C_6H_{14}; [110-54-3]	[172] U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.10	0.9872	0.0128
301.95	0.9843	0.0157
306.20	0.9841	0.0199
311.45	0.9731	0.0269
319.65	0.9574	0.0426
322.65	0.9501	0.0499
331.85	0.9145	0.0855

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Analytical balance and constant-temperature bath.

Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:

(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.

(2) Purity not given, POCh Gliwice, Poland, dried over phosphorous pentoxide and then fractionally distilled before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Heptane; C_7H_{16}; [142-82-5]	[173] U. Domańska and T. Hofman, J. Solution Chem. **14**, 531 (1985). [172] U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
292.15	0.9886	0.0114
296.75	0.9851	0.0149
302.05	0.9803	0.0197
307.35	0.9741	0.0259
311.85	0.9676	0.0324
315.45	0.9605	0.0395
319.15	0.9523	0.0477
323.55	0.9415	0.0585
329.45	0.9271	0.0729
334.85	0.9047	0.0953
341.45	0.8618	0.1382
341.85	0.8449	0.1551

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Analytical balance and constant-temperature bath.

Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:

(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.

(2) Purity not given, VEB Jena Pharm, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[173]U. Domańska and T. Hofman, J. Solution Chem. **14**, 531 (1985). [172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.45	0.9854	0.0146
304.95	0.9721	0.0279
316.65	0.9485	0.0515
319.40	0.9385	0.0615
325.30	0.9115	0.0885
329.35	0.8941	0.1059
333.45	0.8619	0.1381
338.15	0.8152	0.1848

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, POCh Gliwice, Poland, dried over phosphorous pentoxide and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

59.3. 2-Methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Benzene; C_6H_6; [71-43-2]	[172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
294.25	0.9352	0.0648
301.85	0.9049	0.0951
311.85	0.8471	0.1529
323.75	0.7721	0.2279
329.25	0.7186	0.2814
334.85	0.6559	0.3441
338.75	0.6113	0.3887
345.25	0.5389	0.4611

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, POCh Gliwice, Poland, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]	[172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.55	0.9175	0.0825
300.70	0.9063	0.0937
306.60	0.8765	0.1235
311.55	0.8476	0.1524
316.10	0.8224	0.1776
321.90	0.7812	0.2188
323.30	0.7593	0.2407
331.00	0.6954	0.3046
339.90	0.5916	0.4084

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, Reakhim, Poland, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

59.4. 2-Methylbenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8694	0.1306

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8491	0.1509

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8486	0.1514

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8506	0.1494

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8876	0.1124

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

59.5. 2-Methylbenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8282	0.1718

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8852	0.1148

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9061	0.0939

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7371	0.2629

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7466	0.2534

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

59.6. 2-Methylbenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Tetrachloromethane; CCl_4; [56-23-5]	[172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.20	0.9383	0.0617
305.85	0.9017	0.0983
312.05	0.8692	0.1308
318.15	0.8273	0.1727
328.05	0.7492	0.2508
336.35	0.6602	0.3398

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, POCh Gliwice, Poland, dried over phosphorous pentoxide and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Diiodomethane; CH_2I_2; [75-11-6]	[172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
294.45	0.9962	0.00378
301.05	0.9941	0.00588
303.75	0.9926	0.00740
307.45	0.9913	0.00870
308.55	0.9905	0.00948
312.15	0.9886	0.0114
316.45	0.9851	0.0149
321.15	0.9787	0.0213
324.85	0.9733	0.0267
328.35	0.9664	0.0336
332.45	0.9562	0.0438
336.45	0.9401	0.0599
340.45	0.9175	0.0825
343.85	0.8823	0.1177
345.55	0.8614	0.1386

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, Chemapol, CSRS, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	[172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
299.05	0.8517	0.1483
301.05	0.8429	0.1571
305.95	0.8120	0.1880
309.10	0.7796	0.2204
314.70	0.7439	0.2561
319.15	0.7011	0.2989
323.70	0.6582	0.3418
326.85	0.6213	0.3787
334.00	0.5389	0.4611
342.85	0.4295	0.5705
354.15	0.2799	0.7201

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, Intern. Enzymes Limited, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	[172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.05	0.9031	0.0969
302.35	0.8720	0.1280
307.70	0.8410	0.1590
310.80	0.8205	0.1795
318.65	0.7681	0.2319
328.50	0.6828	0.3172
335.25	0.6121	0.3879

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, POCh Gliwice, Poland, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Bromobenzene; C_6H_5Br; [108-86-1]	[172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.35	0.9043	0.0957
301.95	0.8884	0.1116
308.20	0.8526	0.1474
312.65	0.8237	0.1763
317.55	0.7867	0.2133
330.95	0.6773	0.3227
334.60	0.6371	0.3629
344.15	0.5176	0.4824
352.10	0.4063	0.5937

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, POCh Gliwice, Poland, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

59.7. 2-Methylbenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Ethanol; C_2H_6O; [64-17-5]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8599	0.1401

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 3.712 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1460$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Ethanol; C_2H_6O; [64-17-5]	[173]U. Domańska and T. Hofman, J. Solution Chem. **14**, 531 (1985). [172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
291.55	0.8791	0.1209
296.05	0.8665	0.1335
301.65	0.8442	0.1558
306.25	0.8228	0.1772
312.05	0.7973	0.2027
316.05	0.7749	0.2251
319.35	0.7560	0.2440
323.35	0.7301	0.2699
329.35	0.6874	0.3126
336.85	0.6349	0.3651

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, POCh Gliwice, Poland, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Propanol; C_3H_8O; [71-23-8]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8550	0.1450

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2-Propanol; C_3H_8O; [67-63-0]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8388	0.1612

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2-Propanol; C_3H_8O; [67-63-0]	[173]U. Domańska and T. Hofman, J. Solution Chem. **14**, 531 (1985). [172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
292.65	0.8643	0.1357
296.75	0.8457	0.1543
301.95	0.8262	0.1738
306.75	0.8019	0.1981
312.40	0.7723	0.2277
317.75	0.7388	0.2612
324.90	0.6957	0.3043
333.35	0.6337	0.3663
340.15	0.5798	0.4202
344.75	0.5344	0.4656

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, POCh Gliwice, Poland, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8449	0.1551

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8300	0.1700

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8771	0.1229

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2-Methyl-2-propanol; C_3H_8O; [75-65-0]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7862	0.2138

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8354	0.1646

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8144	0.1856

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8619	0.1381

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8527	0.1473

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8293	0.1707

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8265	0.1735

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8245	0.1755

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8242	0.1758

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[77]J. Qingzhu, M. Peisheng, Y. Shouzhi, W. Qiang, W. Chang, and L. Guiju, J. Chem. Eng. Data **53**, 1278 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.15	0.8452	0.1548
299.65	0.8354	0.1646
301.15	0.8195	0.1805
302.65	0.8105	0.1895
304.75	0.8044	0.1956
305.35	0.8033	0.1967
306.25	0.7998	0.2002
306.95	0.7924	0.2076
308.95	0.7806	0.2194
310.65	0.7704	0.2296
312.25	0.7606	0.2394
314.05	0.7501	0.2499
315.75	0.7399	0.2601
316.95	0.7295	0.2705
318.75	0.7193	0.2807
320.35	0.7060	0.2940
321.55	0.6954	0.3046

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating water bath, analytical balance, and laser monitoring system.
Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate 0.5 K/20 min (0.2 K/20 min or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) <99%, Chemical source not specified, used as received.
(2) <99%, Chemical source not specified, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0005.

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8147	0.1853

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

59.8. 2-Methylbenzoic acid solubility data in miscellaneous organic solvents

Components: (1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	**Original Measurements:** [171]R. Coaxum, K. R. Hoover, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 313 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9592	0.04081

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components: (1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	**Original Measurements:** [172]U. Domańska, Pol. J. Chem. **60**, 847 (1986).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
298.35	0.9170	0.0830
299.95	0.9092	0.0908
305.25	0.8853	0.1147
315.00	0.8283	0.1717
321.65	0.7827	0.2173
327.15	0.7373	0.2627
338.35	0.6172	0.3828

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and constant-temperature bath.
Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased. The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:
(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, J. E. London, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error, estimated by compiler).

59.9. 2-Methylbenzoic acid solubility data in binary organic solvent mixtures

Components: (1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Heptane; C_7H_{16}; [142-82-5] (3) Cyclohexane; C_6H_{12}; [110-82-7]	**Original Measurements:** [173]U. Domańska and T. Hofman, J. Solution Chem. **14**, 531 (1985).
Variables: Temperature; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	$x_2^{(s)}$[a]	x_2[b]	x_1[c]
295.45	0.0000	0.0000	0.0146
304.95	0.0000	0.0000	0.0279
316.65	0.0000	0.0000	0.0515
319.40	0.0000	0.0000	0.0615
325.30	0.0000	0.0000	0.0885
329.35	0.0000	0.0000	0.1059
333.45	0.0000	0.0000	0.1381
338.15	0.0000	0.0000	0.1848
292.05	0.1999	0.1976	0.0117
294.85	0.1999	0.1971	0.0140
300.55	0.1999	0.1960	0.0194
304.95	0.1999	0.1948	0.0254
310.95	0.1999	0.1932	0.0336

T/K	$x_2^{(s)a}$	x_2^{b}	x_1^{c}
314.55	0.1999	0.1912	0.0436
319.55	0.1999	0.1888	0.0556
327.15	0.1999	0.1838	0.0805
333.05	0.1999	0.1773	0.1130
338.35	0.1999	0.1699	0.1501
342.55	0.1999	0.1628	0.1855
292.55	0.3988	0.3944	0.0111
297.05	0.3988	0.3931	0.0144
302.85	0.3988	0.3908	0.0200
306.45	0.3988	0.3889	0.0248
311.15	0.3988	0.3859	0.0324
319.55	0.3988	0.3792	0.0491
325.45	0.3988	0.3719	0.0675
330.95	0.3988	0.3621	0.0921
336.65	0.3988	0.3478	0.1280
340.95	0.3988	0.3336	0.1634
292.65	0.5938	0.5867	0.0119
297.85	0.5938	0.5842	0.0161
302.95	0.5938	0.5810	0.0216
308.95	0.5938	0.5759	0.0301
316.25	0.5938	0.5671	0.0449
322.55	0.5938	0.5569	0.0622
329.05	0.5938	0.5427	0.0861
334.85	0.5938	0.5247	0.1163
339.15	0.5938	0.5062	0.1476
343.15	0.5938	0.4861	0.1814
292.95	0.8000	0.7841	0.0119
299.95	0.8000	0.7862	0.0172
305.55	0.8000	0.7811	0.0236
311.35	0.8000	0.7738	0.0327
318.75	0.8000	0.7621	0.0474
324.45	0.8000	0.7500	0.0638
328.95	0.8000	0.7334	0.0832
334.65	0.8000	0.7174	0.1032
337.25	0.8000	0.6964	0.1295
341.35	0.8000	0.6702	0.1622
344.45	0.8000	0.6454	0.1933
292.15	1.0000	0.9886	0.0114
296.75	1.0000	0.9851	0.0149
302.05	1.0000	0.9803	0.0197
307.35	1.0000	0.9741	0.0259
311.85	1.0000	0.9676	0.0324
315.45	1.0000	0.9605	0.0395
319.15	1.0000	0.9523	0.0477
323.55	1.0000	0.9415	0.0585
329.45	1.0000	0.9271	0.0729
334.85	1.0000	0.9047	0.0953
341.45	1.0000	0.8618	0.1382
341.85	1.0000	0.8449	0.1551

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Analytical balance and constant-temperature bath.

Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:

(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.

(2) Purity not given, Chemical source not given, dried over molecular sieves and then fractionally distilled before use.

(3) Purity not given, Chemical source not given, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:

Temperature: ±0.1 K.

$x_2^{(s)}$: ±0.0001.

x_1: ±2.0% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Ethanol; C_2H_6O; [64-17-5] (3) Cyclohexane; C_6H_{12}; [110-82-7]	[173]U. Domańska and T. Hofman, J. Solution Chem. **14**, 531 (1985).
Variables:	**Prepared by:**
Temperature; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	$x_2^{(s)a}$	x_2^{b}	x_1^{c}
295.45	0.0000	0.0000	0.0146
304.95	0.0000	0.0000	0.0279
316.65	0.0000	0.0000	0.0515
319.40	0.0000	0.0000	0.0615
325.30	0.0000	0.0000	0.0885
329.35	0.0000	0.0000	0.1059
333.45	0.0000	0.0000	0.1381
338.15	0.0000	0.0000	0.1848
287.15	0.1999	0.1885	0.0569
294.15	0.1999	0.1852	0.0735
303.15	0.1999	0.1804	0.0975
311.15	0.1999	0.1749	0.1250
313.85	0.1999	0.1719	0.1399
317.65	0.1999	0.1684	0.1576
320.75	0.1999	0.1658	0.1708
325.35	0.1999	0.1603	0.1980
331.15	0.1999	0.1526	0.2366
332.15	0.1999	0.1485	0.2570
286.15	0.4007	0.3675	0.0828
290.15	0.4007	0.3628	0.0946
294.15	0.4007	0.3578	0.1070
297.15	0.4007	0.3533	0.1183
298.45	0.4007	0.3518	0.1221
308.15	0.4007	0.3372	0.1585
311.15	0.4007	0.3294	0.1780
317.05	0.4007	0.3180	0.2064
321.35	0.4007	0.3054	0.2379
324.35	0.4007	0.2968	0.2594
289.35	0.5902	0.5252	0.1101
298.85	0.5902	0.5061	0.1425
303.65	0.5902	0.4955	0.1604
314.65	0.5902	0.4646	0.2128
318.15	0.5902	0.4599	0.2207
319.95	0.5902	0.4466	0.2433
325.15	0.5902	0.4270	0.2766
327.75	0.5902	0.4164	0.2945
288.05	0.8001	0.7049	0.1190
292.15	0.8001	0.6942	0.1324
295.75	0.8001	0.6844	0.1446
299.45	0.8001	0.6718	0.1603

T/K	$x_2^{(s)}$[a]	x_2[b]	x_1[c]
304.05	0.8001	0.6590	0.1763
306.95	0.8001	0.6470	0.1914
312.25	0.8001	0.6315	0.2107
315.85	0.8001	0.6172	0.2286
319.65	0.8001	0.6021	0.2475
323.45	0.8001	0.5626	0.2968
329.55	0.8001	0.5611	0.2987
333.95	0.8001	0.5370	0.3288
291.55	1.0000	0.8791	0.1209
296.05	1.0000	0.8665	0.1335
301.65	1.0000	0.8442	0.1558
306.25	1.0000	0.8228	0.1772
312.05	1.0000	0.7973	0.2027
316.05	1.0000	0.7749	0.2251
319.35	1.0000	0.7560	0.2440
323.35	1.0000	0.7301	0.2699
329.35	1.0000	0.6874	0.3126
336.85	1.0000	0.6349	0.3651

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Analytical balance and constant-temperature bath.

Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:

(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.
(2) Purity not given, Chemical source not given, dried over molecular sieves and then fractionally distilled before use.
(3) Purity not given, Chemical source not given, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:

Temperature: ±0.1 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±2% (relative error, estimated by compiler).

Components:

(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1]
(2) 2-Propanol; C_3H_8O; [67-63-0]
(3) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:

[173]U. Domańska and T. Hofman, J. Solution Chem. **14**, 531 (1985).

Variables:

Temperature; Solvent Composition

Prepared by:

W. E. Acree, Jr.

Experimental Values

T/K	$x_2^{(s)}$[a]	x_2[b]	x_1[c]
295.45	0.0000	0.0000	0.0146
304.95	0.0000	0.0000	0.0279
316.65	0.0000	0.0000	0.0515
319.40	0.0000	0.0000	0.0615
325.30	0.0000	0.0000	0.0885
329.35	0.0000	0.0000	0.1059
333.45	0.0000	0.0000	0.1381
338.15	0.0000	0.0000	0.1848
292.45	0.2000	0.1849	0.0757
296.65	0.2000	0.1828	0.0862
301.75	0.2000	0.1804	0.0982
306.95	0.2000	0.1773	0.1136
311.55	0.2000	0.1735	0.1325
317.25	0.2000	0.1683	0.1585
323.45	0.2000	0.1612	0.1940
328.55	0.2000	0.1535	0.2326
334.55	0.2000	0.1433	0.2834
339.45	0.2000	0.1339	0.3303
343.35	0.2000	0.1258	0.3712
290.95	0.4000	0.3566	0.1085
293.25	0.4000	0.3538	0.1156
298.45	0.4000	0.3479	0.1303
301.85	0.4000	0.3416	0.1459
307.95	0.4000	0.3337	0.1658
312.65	0.4000	0.3248	0.1881
318.85	0.4000	0.3120	0.2199
325.75	0.4000	0.2950	0.2625
332.45	0.4000	0.2757	0.3108
338.35	0.4000	0.2564	0.3590
343.15	0.4000	0.2412	0.3970
291.15	0.6000	0.5236	0.1274
295.75	0.6000	0.5129	0.1452
300.75	0.6000	0.5003	0.1662
306.55	0.6000	0.4859	0.1901
311.35	0.6000	0.4712	0.2147
318.05	0.6000	0.4516	0.2473
324.45	0.6000	0.4283	0.2863
331.25	0.6000	0.3997	0.3339
336.55	0.6000	0.3761	0.3731
342.55	0.6000	0.3452	0.4246
291.25	0.8001	0.6940	0.1326
298.45	0.8001	0.6794	0.1509
302.45	0.8001	0.6594	0.1759
307.45	0.8001	0.6407	0.1992
312.45	0.8001	0.6214	0.2234
317.85	0.8001	0.5988	0.2516
323.25	0.8001	0.5749	0.2815
329.65	0.8001	0.5411	0.3237
337.15	0.8001	0.5006	0.3743
341.15	0.8001	0.4768	0.4041
292.65	1.0000	0.8643	0.1357
296.75	1.0000	0.8457	0.1543
301.95	1.0000	0.8262	0.1738
306.75	1.0000	0.8019	0.1981
312.40	1.0000	0.7723	0.2277
317.75	1.0000	0.7388	0.2612
324.90	1.0000	0.6957	0.3043
333.35	1.0000	0.6337	0.3663
340.15	1.0000	0.5798	0.4202
344.75	1.0000	0.5344	0.4656

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Analytical balance and constant-temperature bath.

Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:

(1) 99+%, Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.

(2) Purity not given, Chemical source not given, dried over molecular sieves and then fractionally distilled before use.

(3) Purity not given, Chemical source not given, dried over molecular sieves and then fractionally distilled before use.

Estimated Error:

Temperature: ±0.1 K.

$x_2^{(s)}$: ±0.0001.

x_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Methylbenzoic acid; $C_8H_8O_2$; [118-90-1] (2) Diiodomethane; CH_2I_2; [75-11-6] (3) Cyclohexane; C_6H_{12}; [110-82-7]	[174]U. Domańska, J. Solution Chem. **18**, 1153 (1989).
Variables:	**Prepared by:**
Temperature; Solvent Composition	W. E. Acree, Jr.

Experimental Values

T/K	$x_2^{(s)}$[a]	x_2[b]	x_1[c]
295.45	0.0000	0.0000	0.0146
304.95	0.0000	0.0000	0.0279
316.65	0.0000	0.0000	0.0515
319.40	0.0000	0.0000	0.0615
325.30	0.0000	0.0000	0.0885
329.35	0.0000	0.0000	0.1059
333.45	0.0000	0.0000	0.1381
338.15	0.0000	0.0000	0.1848
290.75	0.2000	0.1954	0.0228
293.35	0.2000	0.1947	0.0265
295.35	0.2000	0.1939	0.0306
297.95	0.2000	0.1930	0.0350
301.35	0.2000	0.1915	0.0425
304.25	0.2000	0.1897	0.0516
306.95	0.2000	0.1881	0.0595
309.25	0.2000	0.1862	0.0691
312.95	0.2000	0.1818	0.0909
316.55	0.2000	0.1804	0.0979
318.45	0.2000	0.1767	0.1164
322.05	0.2000	0.1717	0.1416
327.25	0.2000	0.1626	0.1869
330.75	0.2000	0.1540	0.2299
334.45	0.2000	0.1446	0.2769
338.05	0.2000	0.1336	0.3318
342.95	0.2000	0.1196	0.4021
346.05	0.2000	0.1093	0.4537
349.45	0.2000	0.0989	0.5054
294.85	0.3975	0.3853	0.0308
298.25	0.3975	0.3822	0.0386
301.55	0.3975	0.3785	0.0477
304.95	0.3975	0.3746	0.0577
307.65	0.3975	0.3705	0.0678
310.45	0.3975	0.3661	0.0789
313.55	0.3975	0.3616	0.0903
318.25	0.3975	0.3524	0.1134
322.65	0.3975	0.3426	0.1381
327.45	0.3975	0.3259	0.1801
332.15	0.3975	0.3080	0.2252
336.35	0.3975	0.2894	0.2720
341.75	0.3975	0.2647	0.3342
351.15	0.3975	0.2152	0.4586
294.35	0.5002	0.4862	0.0280
298.55	0.5002	0.4812	0.0379
302.55	0.5002	0.4759	0.0486
307.95	0.5002	0.4687	0.0630
311.65	0.5002	0.4604	0.0796
316.15	0.5002	0.4494	0.1016
320.85	0.5002	0.4374	0.1255
325.35	0.5002	0.4210	0.1583
329.05	0.5002	0.4049	0.1905
332.85	0.5002	0.3873	0.2258
335.55	0.5002	0.3701	0.2600
342.15	0.5002	0.3305	0.3393
296.85	0.6002	0.5830	0.0287
302.45	0.6002	0.5755	0.0411
308.35	0.6002	0.5649	0.0588
312.75	0.6002	0.5550	0.0753
316.85	0.6002	0.5440	0.0937
318.85	0.6002	0.5349	0.1088
323.25	0.6002	0.5235	0.1278
323.75	0.6002	0.5121	0.1467
328.05	0.6002	0.5002	0.1666
331.35	0.6002	0.4821	0.1967
334.75	0.6002	0.4606	0.2326
337.45	0.6002	0.4395	0.2677
342.45	0.6002	0.3988	0.3356
346.95	0.6002	0.3595	0.4011
293.85	0.7999	0.7877	0.0152
299.35	0.7999	0.7838	0.0201
304.05	0.7999	0.7777	0.0277
311.65	0.7999	0.7673	0.0408
314.65	0.7999	0.7589	0.0512
320.05	0.7999	0.7477	0.0653
324.45	0.7999	0.7335	0.0830
328.55	0.7999	0.7152	0.1059
333.65	0.7999	0.8587	0.1413
337.55	0.7999	0.6562	0.1797
342.95	0.7999	0.6029	0.2463
348.55	0.7999	0.5223	0.3471
294.45	1.0000	0.9962	0.00378
301.05	1.0000	0.9941	0.00588
303.75	1.0000	0.9926	0.00740
307.45	1.0000	0.9913	0.00870
308.55	1.0000	0.9905	0.00948
312.15	1.0000	0.9886	0.0114
316.45	1.0000	0.9851	0.0149
321.15	1.0000	0.9787	0.0213
324.85	1.0000	0.9733	0.0267
328.35	1.0000	0.9664	0.0336
332.45	1.0000	0.9562	0.0438
336.45	1.0000	0.9401	0.0599
340.45	1.0000	0.9175	0.0825
343.85	1.0000	0.8823	0.1177
345.55	1.0000	0.8614	0.1386

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.

[b] x_2: mole fraction of component 2 in the saturated solution.

[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Analytical balance and constant-temperature bath.

Solubilities were determined by a dynamic method. Weighed amounts of solute and solvent were placed in sample container and placed in a constant-temperature bath. The temperature of the bath was slowly increased (2 K/h near the equilibrium temperature). The temperature at which the last crystals disappeared was taken as the temperature of the solution-crystal equilibrium.

Source and Purity of Chemicals:

(1) Analytical grade, Fluka Chemicals, Switzerland, purified by double vacuum sublimation.

(2) Purity not given, Chemapol, Czechoslovakia, used as received.

(3) 99.9%, Chemical source not given, dried over phosphorous pentoxide and then fractionally distilled before use.

Estimated Error:

Temperature: ±0.1 K.

$x_2^{(s)}$: ±0.0001.

x_1: ±0.0005.

60. Solubility of 3-Methylbenzoic Acid in Organic Solvents

60.1. Critical evaluation of experimental solubility data

There have been several published studies[14,49,54,63,72,77,130] investigating the solubility behavior of 3-methylbenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Daniels *et al.*[14] measured the solubility of 3-methylbenzoic acid in 18 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, and 1-decanol), in one dialkyl ether (1,1′-oxybisethane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in three alkanoates (methyl ethanoate, ethyl ethanoate, and butyl ethanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to calculate the Abraham solute descriptors of 3-methylbenzoic acid. The authors were able to assemble a total of 42 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 3-methylbenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -2.14$.[131,132,176] The McGowan volume of 3-methylbenzoic acid, $V = 1.0726$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.730$. This left four solute descriptors (*S*, *A*, *B*, and *L*) still to be determined. The 42 equations were then solved using the Microsoft "SOLVER" program to yield numerical values of the remaining four solute descriptors, $S = 0.890$, $A = 0.600$, $B = 0.400$, and $L = 4.8187$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -7.120$ for the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.077 and 0.083 $\log_{10}$ units, respectively.

TABLE 44. Comparison between observed and calculated molar solubilities of 3-methylbenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp,a}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Methanol	0.437	0.369	0.345
Ethanol	0.371	0.399	0.389
1-Propanol	0.292	0.296	0.300
2-Propanol	0.292	0.315	0.333
1-Butanol	0.217	0.206	0.215
2-Butanol	0.288	0.258	0.241
2-Methyl-1-propanol	0.145	0.161	0.140
2-Methyl-2-propanol	0.353	0.325	0.371
1-Pentanol	0.204	0.219	0.224
2-Pentanol	0.244	0.254	0.239
3-Methyl-1-butanol	0.164	0.192	0.158
1-Hexanol	0.166	0.170	0.164
1-Heptanol	0.141	0.130	0.134
1-Octanol	0.119	0.070	0.024
1-Decanol	−0.044	0.022	0.027
1,1′-Oxybisethane	0.242	0.072	0.127
Tetrahydrofuran	0.545	0.664	0.638
1,4-Dioxane	0.303	0.342	0.333
Methyl ethanoate	0.203	0.069	0.050
Ethyl ethanoate	0.136	0.130	0.125
Butyl ethanoate	−0.016	0.004	−0.026

[a] Experimental data were taken from Daniels *et al.*[14]

After the 3-methylbenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, methyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 3-methylbenzoic acid solubility data. Table 44 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 3-methylbenzoic acid, x_1, determined by Daniels *et al.*[14] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1V_1+(1-x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 3-methylbenzoic acid is $V_{\mathrm{solute}} = 121.8\ \mathrm{cm}^3\ \mathrm{mol}^{-1}$. Examination of the numerical entries in Table 44 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

Qingzhu *et al.*[77] measured the solubility of 3-methylbenzoic acid in 1-octanol as a function of temperature using a dynamic method with laser monitoring to observe when dissolution was complete. The calculated curve-fit parameters from the Buchowski λh-model [see Eq. (9)] of $\lambda = 0.7617$ and

$h = 2624.62$ described the observed solubility data to within a mean relative deviation of 0.8%.

The experimental solubility data for 3-methylbenzoic acid in organic solvents are in Secs. 60.2–60.9.

60.2. 3-Methylbenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components: (1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Hexane; C_6H_{14}; [110-54-3]	**Original Measurements:** [49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9883	0.0117

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was recrystallized twice from aqueous-ethanol and dried at 353 K before use.
(2) 99%, Chemical source not given, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

Components: (1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	**Original Measurements:** [54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9821	0.0179

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

Components: (1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	**Original Measurements:** [49]W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9873	0.0127

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was recrystallized twice from aqueous-ethanol and dried at 353 K before use.
(2) 99%, Chemical source not given, stored over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
x_1: ±1% (relative error).

60.3. 3-Methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.894	0.106

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

60.4. 3-Methylbenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8636	0.1364

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8609	0.1391

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8737	0.1263

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8820	0.1180

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

60.5. 3-Methylbenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8111	0.1889

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.6671	0.3329

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.627	0.373

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.

(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:

Temperature: ±0.02 K.

x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8140	0.1860

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.709	0.291

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.

Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:

(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.

(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:

Temperature: ±0.02 K.

x_1: ±1.0% (relative error).

60.6. 3-Methylbenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Methanol; CH_4O; [67-56-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8570	0.1430

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Ethanol; C_2H_6O; [64-17-5]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8383	0.1617

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 4.187 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1616$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8382	0.1618

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Propanol; C_3H_8O; [67-63-0]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8347	0.1653

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8405	0.1595

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8105	0.1895

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8655	0.1345

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7733	0.2267

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8227	0.1773

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8035	0.1965

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8530	0.1470

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8368	0.1632

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8172	0.1828

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8332	0.1668

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7867	0.2133

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8090	0.1910

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8015	0.1985

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[77]J. Qingzhu, M. Peisheng, Y. Shouzhi, W. Qiang, W. Chang, and L. Guiju, J. Chem. Eng. Data **53**, 1278 (2008).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.25	0.8259	0.1741
297.25	0.8212	0.1788
299.15	0.8144	0.1856
300.25	0.8063	0.1937
302.90	0.8011	0.1989
303.80	0.7906	0.2094
305.85	0.7806	0.2194
308.45	0.7687	0.2313
311.75	0.7543	0.2470
313.80	0.7379	0.2621
316.25	0.7251	0.2749
317.65	0.7133	0.2867
322.15	0.6945	0.3055

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating water bath, analytical balance, and laser monitoring system. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate of 0.5 K/20 min (0.2 K/20 min or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) <99%, Chemical source not specified, used as received.
(2) <99%, Chemical source not specified, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0005.

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[14]C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8370	0.1630

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

60.7. 3-Methylbenzoic acid solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7894	0.2106

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7894	0.2106

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/ visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7726	0.2274

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/ visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7835	0.2165

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Constant-temperature bath, calorimetric thermometer, and an ultraviolet/ visible spectrophotometer.

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:

(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.

(2) 99+%, Acros Organics, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:

Temperature: ±0.1 K.

x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7945	0.2055

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) 1-Methyl-2-*tert*-butoxyethanol; $C_7H_{16}O_2$; [57018-52-7]	[130] L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.7743	0.2257

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

60.8. 3-Methylbenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[14] C. R. Daniels, A. K. Charlton, R. M. Wold, W. E. Acree, Jr., and M. H. Abraham, Can. J. Chem. **81**, 1492 (2003).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9611	0.03892

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 279 nm.

Source and Purity of Chemicals:
(1) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

60.9. 3-Methylbenzoic acid solubility data in binary organic solvent mixtures

Components:	**Original Measurements:**
(1) 3-Methylbenzoic acid; $C_8H_8O_2$; [99-04-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Hexane; C_6H_{14}; [110-54-3]	[49] W. E. Acree, Jr. and G. L. Bertrand, J. Pharm. Sci. **70**, 1033 (1981).
Variables: T/K = 298.15; Solvent Composition	**Prepared by:** W. E. Acree, Jr.

Experimental Values

$x_2^{(s)a}$	x_2^{b}	x_1^{c}
0.0000	0.0000	0.0117
0.2380	0.2350	0.0127
0.4028	0.3974	0.0133
0.6121	0.6037	0.0137
0.8239	0.8127	0.0136
1.0000	0.9873	0.0127

[a] $x_2^{(s)}$: initial mole fraction of component 2 in the binary solvent mixture.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature water bath and an analytical balance.
Excess solute and solvent and were placed in brown glass containers and allowed to equilibrate in a constant-temperature water bath for several days. Attainment of equilibrium was verified by repetitive measurements after several additional days. Solubility was determined by transferring a weighed aliquot through a coarse filter into a flask containing blank nonaqueous titration solvent. The solutions were titrated with freshly standardized sodium methoxide to the thymol blue endpoint.

Source and Purity of Chemicals:
(1) 99%, Chemical source not given, was recrystallized twice from aqueous ethanol and dried at 353 K before use.
(2) 99+%, Chemical source not given, was dried over molecular sieves and distilled before use.
(3) 99%, Chemical source not given, was dried over molecular sieves and distilled before use.

Estimated Error:
Temperature: ±0.01 K.
$x_2^{(s)}$: ±0.0001.
x_1: ±1% (relative error).

61. Solubility of 4-Methylbenzoic Acid in Organic Solvents

61.1. Critical evaluation of experimental solubility data

There have been several published studies[54,60,63,72,77,82,84,85,177–179] investigating the solubility behavior of 4-methylbenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Hancock *et al.*[54,63] measured the solubility of 4-methylbenzoic acid in cyclohexane, benzene, tetrahydrofuran, and 1,4-dioxane at 303 K. Thuaire[72] determined the solubility of 4-methylbenzoic acid in ethanol as part of study involving solubilities of benzoic acids in binary aqueous-ethanol solvent mixtures. It is not possible to perform a critical evaluation of the experimental data as both research groups performed measurements at only a single temperature, and there are no independent experimental solubility data for 4-methylbenzoic acid in these five solvents.

There have been several experimental studies[60,77,84,177–179] examining the solubility of 4-methylbenzoic acid in different organic solvents as a function of temperature. Luo *et al.*[179] determined the solubility of 4-methylbenzoic acid in ethanoic acid and in binary aqueous-ethanoic acid mixtures at several temperatures between 303 and 363 K as part of an experimental study aimed at calculating UNIFAC model group parameters for the ArCOOH group (carboxylic acid group connected to an aromatic ring) interacting with an aliphatic COOH group, with aliphatic CH_3 and CH_2 groups, with an aromatic CH_3 group and with an aromatic ArH group. The authors used the Modified Apelblat equation [Eq. (8); $A = -11.717$, $B = -1729.0$, and $C = 3.2722$] to describe the variation in the mole fraction solubility with temperature to within a mean relative deviation of 2.75%. Zhao *et al.*[60] measured the solubility of 4-methylbenzoic acid in isobutyl ethanoate at 22 temperatures between 300 and 348 K. The experimental data were correlated with the Wilson and UNIQUAC models. Interaction coefficients calculated from the experimental solid-liquid equilibrium data provided a reasonably accurate mathematical description of the measured values. The mean absolute relative deviation between calculated and observed values was 4.76% (Wilson model) and 5.74% (UNIQUAC model).

Qingzhu *et al.*[77] measured the solubility of 4-methylbenzoic acid in 1-octanol using a dynamic method with laser monitoring to observe when dissolution was complete. The calculated curve-fit parameters from the Buchowski λh-model [see Eq. (9)] of $\lambda = 0.7326$ and $h = 2940.14$ described the observed solubility data to within a mean relative deviation of 0.7%.

Li *et al.*[84] determined the solubility of 4-methylbenzoic acid in *N*-methyl-2-pyrrolidone from 296 to 370 K using a synthetic method with laser monitoring to determine when the last amount of solid solute dissolved. The authors employed a polynomial expression in temperature

$$x_1 = -32.6862 + 0.30878\,T - 9.78125 \times 10^{-4}\,T + 10.4307 \times 10^{-7}T^2 \qquad (65)$$

to represent the measured mole fraction solubility data. The root-mean-square deviation between the observed x_1 data and calculated values from Eq. (65) was on the order of 0.0052 mole fraction.

The experimental solubility data for 4-methylbenzoic acid in different organic solvents are in Secs. 61.2–61.7.

61.2. 4-Methylbenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54] C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9975	0.00249

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

61.3. 4-Methylbenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9908	0.00920

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]	[177]Q. Kong, Y. Cheng, X. Bao, L. Wang, and X. Li, Fluid Phase Equilib. **340**, 46 (2013).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.2	0.9867	0.01332
308.2	0.9847	0.01525
313.2	0.9822	0.01776
318.2	0.9766	0.02338
323.2	0.9716	0.02840
328.2	0.9646	0.03544
333.2	0.9578	0.04217
338.2	0.9467	0.05326
343.2	0.9308	0.06917
348.2	0.9217	0.07825
353.2	0.9144	0.08555

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Thermostatic circulating water bath, analytical balance, jacketed equilibrium glass vessel, and a high-performance liquid chromatographic system equipped with uv absorbance detector.
Solubility was measured by a static analytical method. Excess solute and solvent were placed in a jacketed equilibrium glass vessel and allowed to equilibrate at constant temperature for at least 36 h. Samples of the clear saturated solution was removed by syringe and transferred to a tared test tube containing 3 ml of methanol. The test tube with sample was then weighed. The concentration of the 4-methylbenzoic acid in the saturated solution was determined in triplicate by chromatographic analysis (hplc).

Source and Purity of Chemicals:
(1) 99+%, Shanghai Fe Xiang Chemical Company, Shanghai, China, used as received.
(2) 99%, Sinopharm Chemical Reagent Co., Ltd., China, used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error).

61.4. 4-Methylbenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) Isobutyl ethanoate; $C_6H_{12}O_2$; [110-19-0]	[60]S. Zhao, X. Chen, Q. Dai, and L. Wang, J. Chem. Eng. Data **56**, 2399 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
300.19	0.9672	0.0328
303.04	0.9662	0.0338
306.43	0.9644	0.0356
310.28	0.9579	0.0421
312.70	0.9566	0.0434
315.36	0.9525	0.0475
319.97	0.9475	0.0525
323.16	0.9427	0.0573
324.84	0.9388	0.0612
325.76	0.9347	0.0653
329.67	0.9308	0.0692
332.48	0.9265	0.0735
333.91	0.9226	0.0774
335.96	0.9187	0.0813
337.49	0.9152	0.0848
339.46	0.9115	0.0885
341.07	0.9082	0.0918
342.68	0.9046	0.0954
344.69	0.9006	0.0994
345.82	0.8969	0.1031
347.26	0.8933	0.1067
348.41	0.8900	0.1100

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, thermoelectric circulating water temperature controller, electromagnetic stirrer, analytical balance, and laser monitoring system.
Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate of 1–2 K/h (0.5–1.0 K/h or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.
(2) Analytical Reagent grade, Sinopharm Chemical Reagent Co. Ltd., China, was used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0006.

61.5. 4-Methylbenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.834	0.166

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.904	0.096

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

61.6. 4-Methylbenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 1.202 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.05247$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[77]J. Qingzhu, M. Peisheng, Y. Shouzhi, W. Qiang, W. Chang, and L. Guiju, J. Chem. Eng. Data **53**, 1278 (2008).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.35	0.9405	0.0595
298.05	0.9392	0.0608
298.95	0.9382	0.0618
301.65	0.9337	0.0663
307.25	0.9233	0.0767
308.65	0.9211	0.0789
309.65	0.9184	0.0816
312.95	0.9129	0.0871
314.35	0.9104	0.0896
315.80	0.9075	0.0925
317.65	0.9038	0.0962
319.65	0.9003	0.0997
320.40	0.8990	0.1010
321.55	0.8971	0.1029
322.15	0.8960	0.1040

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating water bath, analytical balance, and laser monitoring system. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate 0.5 K/20 min (0.2 K /20 min or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) <99%, Chemical source not specified, used as received.
(2) <99%, Chemical source not specified, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0005.

61.7. 4-Methylbenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[178]M. Chen and P. Ma, J. Chem. Eng. Data **49**, 756 (2004).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
291.95	0.9658	0.03421
292.45	0.9656	0.03440
297.35	0.9628	0.03724
301.65	0.9599	0.04006
307.75	0.9551	0.04488
311.95	0.9517	0.04829
318.25	0.9449	0.05505
324.95	0.9360	0.06397
328.25	0.9313	0.06868
335.05	0.9177	0.08225
340.45	0.9037	0.09625
344.45	0.8907	0.1093
348.85	0.8730	0.1270
349.75	0.8697	0.1303

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Titanium solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a dynamic method. Weighed amounts of solute and solvent were sealed in a titanium solid-liquid equilibrium cell, and the temperature slowly increased until the solid phase completely disappeared. Near the solid-liquid equilibrium temperature, the rate of temperature increase was 0.1 K/10 min. The disappearance of the solid solute was detected by a laser monitoring system.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) Ethanoic acid; $C_2H_4O_2$; [64-19-7]	[179]W. Luo, Q. Wang, L. Fu, W. Deng, X. Zhang, and C. Guo, Ind. Eng. Chem. Res. **50**, 4099 (2011).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
303.2	0.9616	0.03839
313.2	0.9529	0.04710
323.2	0.9383	0.06174
333.2	0.9182	0.08177
343.2	0.8935	0.1065
353.2	0.8649	0.1351
363.2	0.8333	0.1667

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Jacketed equilibrium glass bottle, analytical balance and thermostatic water-circulator bath.
Excess solute and solvent were placed in a jacketed equilibrium glass bottle and allowed to equilibrate for at least 24 h at constant temperature. For the experimental methodology for determining the concentration of the dissolved solute, the authors reference a paper involving the solubility of 1,4-benzenedicarboxylic acid [Q. B. Wang, H. B. Xu, and X. Li, J. Chem. Eng. Data **50**, 258 (2005)]. In the referenced paper the concentration of the solute was determined by a high-performance liquid chromatographic method of analysis.

Source and Purity of Chemicals:
(1) 99.9%, Shanghai Fine Chemical Reagent Company, China, no purification details were provided.
(2) Analytical Reagent grade, Hangzhou Chemical Reagent Company, China, was used as received.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) *N*,*N*-Dimethylformamide; C_3H_7NO; [64-19-7]	[82]L. Dian-Qing, L. Jiang-Chu, Liu Da-Zhuang, and W. Fu-An, Fluid Phase Equilib. **200**, 69 (2002).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.65	0.8815	0.1185
298.75	0.8691	0.1309
303.05	0.8509	0.1491
307.55	0.8311	0.1689
311.05	0.8131	0.1869
315.55	0.7895	0.2105
320.45	0.7592	0.2408
324.55	0.7325	0.2675
326.85	0.7142	0.2858
328.95	0.6989	0.3011
331.65	0.6759	0.3241
333.05	0.6631	0.3369
335.05	0.6435	0.3565
335.55	0.6364	0.3636

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:

(1) 98.5% (starting purity), Chemical source not given, was an industrial product purified by extracting with trichloromethane, and then recrystallized successively from acetic acid and water. Final purity was 99.7%.

(2) Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:

Temperature: ±0.05 K (estimated by compiler).

x_1: ±0.0005 or less.

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) *N*-Methyl-2-pyrrolidone; C_5H_9NO; [872-50-4]	[84]D.-Q. Li, D.-Z. Liu, and F.-A. Wang, J. Chem. Eng. Data **46**, 172 (2001).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
295.65	0.9321	0.0679
298.65	0.9255	0.0745
303.35	0.9134	0.0866
308.55	0.8997	0.1013
313.75	0.8825	0.1175
319.55	0.8612	0.1388
323.45	0.8458	0.1542
328.75	0.8253	0.1747
334.85	0.7962	0.2038
340.25	0.7699	0.2301
343.35	0.7526	0.2474
346.65	0.7337	0.2663
351.45	0.7034	0.2966
355.75	0.6721	0.3279
360.65	0.6295	0.3705
364.05	0.5900	0.4100
366.55	0.5547	0.4453
369.25	0.5149	0.4851
370.05	0.4995	0.5005

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Jacketed solid-liquid equilibrium cell, analytical balance, magnetic stirring system, temperature controlling system, and a laser monitoring system. Solubilities were determined using a synthetic method. Weighed amounts of solute and solvent were sealed in a jacketed equilibrium vessel, and the temperature slowly increased until the solid phase completely disappeared. The disappearance of the solid solute was detected by a laser monitoring system. Measurements were repeated two or three times to check the reproducibility.

Source and Purity of Chemicals:

(1) 98.5% (starting purity), Chemical source not given, was an industrial product purified by extracting with trichloromethane, and then recrystallized successively from acetic acid and water. Final purity was 99.7%.

(2) 99.0%, Analytical Reagent, Shanghai Chemical Reagent Company, used as received.

Estimated Error:

Temperature: ±0.05 K (estimated by compiler).

x_1: ±0.0005 or less.

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) 5-Methyl-2-thiophenecarboxylic acid; $C_6H_6O_2S$; [1918-79-2]	[85]K. Mislow, J. Phys. Coll. Chem. **52**, 729 (1948).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

t/°C (thawing)	t/°C (melting)	w_1[a]
138	139	0.000
116.6	133.2	0.094
117.0	130.4	0.192
116.2	127.4	0.270
115.6	144.4	0.450
116.2	147.0	0.500
116.4	151.8	0.600
116.2	159.0	0.703
116.8	165.4	0.795
154.2	173.4	0.900
177	178	1.000

[a]w_1: mass fraction solubility of the solute.

The author reports that the binary system forms a simple eutectic at $w_1 = 0.250$ and $t = 116$ °C, with an indication of solid solution formation at $w_1 > 0.80$.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental method involved observing the thawing-melting behavior of binary mixtures of known composition. Thoroughly mixed samples were placed in capillaries and sealed at one end. The capillaries were placed next to the junction of a thermocouple in a hot stage, which was mounted on a polarizing microscope. Heating rates were kept at (2 ± 1)°C/min. The thawing temperature was observed by reflected light, while the melting points were observed by transmitted light. Accuracy of the method, as judged by the reproducibility of the measured data, was estimated to be ±2 °C for thawing and melting temperatures.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, recrystallized from aqueous solution.
(2) Purity not given, Prepared by the authors, synthesized by heating levulinic acid with phosphorous trisulfide to give 2-methylthiophene. Iodination of 2-methylthiophene yielded 5-iodo-2-methylthiophene, which was converted to 5-methyl-2-thiophenecarboxylic acid by the Grignard synthesis.

Estimated Error:
Temperature: 2 °C.
w_1: ±0.002 (estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Methylbenzoic acid; $C_8H_8O_2$; [100-09-4] (2) 5-Bromo-2-thiophenecarboxylic acid; $C_5H_3BrO_2S$; [7311-63-9]	[85]K. Mislow, J. Phys. Coll. Chem. **52**, 729 (1948).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

t/°C (thawing)	t/°C (melting)	w_1[a]
140	141	0.000
134.2	139.6	0.066
134.2	138.2	0.190
133.6	146.2	0.285
133.8	150.6	0.398
135.2	157.0	0.491
135.4	162.0	0.580
134.6	168.8	0.696
154.2	175.8	0.869
177	178	1.000

[a]w_1: mass fraction solubility of the solute.

The author reports that the binary system forms a simple eutectic at $w_1 = 0.140$ and t = 116 °C, with an indication of solid solution formation at $w_1 > 0.75$.

Auxiliary Information

Method/Apparatus/Procedure:
Experimental method involved observing the thawing-melting behavior of binary mixtures of known composition. Thoroughly mixed samples were placed in capillaries and sealed at one end. The capillaries were placed next to the junction of a thermocouple in a hot stage, which was mounted on a polarizing microscope. Heating rates were kept at (2 ± 1)°C/min. The thawing temperature was observed by reflected light, while the melting points were observed by transmitted light. Accuracy of the method, as judged by the reproducibility of the measured data, was estimated to be ±2 °C for thawing and melting temperatures.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, recrystallized from aqueous solution.
(2) Purity not given, Prepared by the authors, synthesized by direct bromination of 2-thiophene-carboxylic acid in glacial acetic acid.

Estimated Error:
Temperature: 2 °C.
w_1: ±0.002 (estimated by compiler).

62. Solubility of 2-Nitrobenzoic Acid in Organic Solvents

62.1. Critical evaluation of experimental solubility data

There have been several published studies[72,77,83,126,127,180,181] investigating the solubility behavior of 2-nitrobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Kolthoff and co-workers[83,181] measured the solubility of 2-nitrobenzoic acid in both methanol and ethanenitrile at 298 K. Biswas *et al.*[126] and Thuaire[72] both determined the solubility in ethanol at 298 K. Sidgwick and Ewbank[127] measured the solubility of 2-nitrobenzoic acid in benzene. Collett and Lazzell[180] later performed solubility measurements for 2-nitrobenzoic acid in benzene, 1,1′-oxybisethane, trichloromethane, and propanone. The internal consistency of the five datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 45, along with the MRD calculated according to Eq. (24). The largest MRD occurs in the 2-nitrobenzoic acid – benzene system, and corresponds to about a 11.5% error in back-calculating the observed mole fraction solubilities.

TABLE 45. Parameters of the Modified Apelblat equation for describing the solubility of 2-nitrobenzoic acid in various organic solvents

Solvent	A	B	C	MRD (%)
Benzene[a]	−149.976	112.67	24.905	11.44
Benzene[b]	−172.585	112.116	28.700	9.46
1,1′-Oxybisethane[b]	−38.774	−0.878	6.420	3.23
Trichloromethane[b]	−123.562	−7.489	20.558	7.19
Propanone[b]	−26.429	−0.573	4.190	2.22

[a] Calculated from the dataset of Sidgwick and Ewbank.[127]

[b] Calculated from the dataset of Collett and Lazzell.[180] For benzene, the first and last data points were removed from the regression analysis in order to obtain a reasonable mathematical representation.

The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point, to changes in the liquid phase composition due to solvent evaporation into the vapor phase, and the large range covered by the experimental values, $x_1 = 0.00142$ to $x_1 = 0.8501$. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 2-nitrobenzoic acid in organic solvents are in Secs. 62.2–62.7.

62.2. 2-Nitrobenzoic acid solubility data in aromatic hydrocarbons

Components:	Original Measurements:
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Benzene; C_6H_6; [71-43-2]	[127] N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
336.2	0.990	0.00993
351.8	0.976	0.0242
363.7	0.951	0.0494
379.0	0.844	0.156
386.2	0.679	0.321
401.5	0.334	0.666

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 420.0 K.

(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Benzene; C_6H_6; [71-43-2]	[180] A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.7	0.9986	0.00142
365.4	0.9501	0.0499
372.4	0.9130	0.0870
381.9	0.7906	0.2094
387.9	0.6608	0.3392
392.9	0.5415	0.4585
396.4	0.4539	0.5461
401.4	0.3574	0.6426
412.0	0.1499	0.8501

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:

(1) Certified Pure, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized twice from aqueous solution. Melting point temperature of purified sample was 420.9 K.

(2) Thiophene-free, Kahlbaum, was dried over sodium and distilled before use.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

62.3. 2-Nitrobenzoic acid solubility data in ethers

Components:	Original Measurements:
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[180] A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
305.9	0.8775	0.1225
329.0	0.7719	0.2281
377.3	0.4919	0.5081
381.1	0.4648	0.5352
396.7	0.3183	0.6817
408.4	0.1710	0.8290

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Certified Pure, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized twice from aqueous solution. Melting point temperature of purified sample was 420.9 K.

(2) U.S.P. grade, Chemical source not given, was washed three times with distilled water, dried over calcium chloride, and distilled twice before use.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

62.4. 2-Nitrobenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	Original Measurements:
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[180] A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
337.4	0.9789	0.0211
357.4	0.9450	0.0550
374.5	0.8306	0.1694
379.4	0.7626	0.2374
387.3	0.6165	0.3835
392.1	0.5137	0.4863
394.4	0.4573	0.5427
398.2	0.4081	0.5919
399.2	0.3928	0.6072
404.0	0.2888	0.7112
405.1	0.2760	0.7240
413.1	0.1199	0.8801

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Certified Pure, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized twice from aqueous solution. Melting point temperature of purified sample was 420.9 K.

(2) Certified Pure, Merck Chemical Company, dried over calcium chloride and distilled twice before use.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

62.5. 2-Nitrobenzoic acid solubility data in alcohols

Components:	Original Measurements:
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Methanol; CH_4O; [67-56-1]	[181] I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 2.99 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by the conductance method.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, refluxed over silver oxide, distilled and dehydrated with magnesium.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Ethanol; C_2H_6O; [64-17-5]	[126]P. K. Biswas, S. C. Lahiri, and B. P. Dey, Bull. Chem. Soc. Jpn. **66**, 2785 (1993).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
1.6261	0.8945	0.1055

[a] c_1: solubility of the solute expressed in units of mol dm^{-3}.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and an ultraviolet/visible spectrophotometer.
Solutions containing excess solute and solvent were allowed to equilibrate at constant temperature for at least 24 h. An aliquot of the saturated solution was removed, filtered, and the absorbance recorded. Solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Puris grade, Fluka Chemicals, recrystallized from aqueous ethanol mixture and dried in an air oven at 390 K. The purified compound was stored in vacuum desiccators.
(2) Absolute, B.C.P.W., Calcutta, India, was distilled twice before use.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±1.0% (relative error, estimated by compiler).
x_1: ±2.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 4.516 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1722$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[77]J. Qingzhu, M. Peisheng, Y. Shouzhi, W. Qiang, W. Chang, and L. Guiju, J. Chem. Eng. Data **53**, 1278 (2008).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.15	0.9239	0.0761
299.65	0.9194	0.0806
300.15	0.9160	0.0840
302.05	0.9105	0.0895
303.15	0.9072	0.0928
306.15	0.8989	0.1011
307.15	0.8955	0.1045
308.35	0.8921	0.1079
309.25	0.8873	0.1127
310.15	0.8828	0.1172
311.75	0.8781	0.1219
313.15	0.8710	0.1290
314.85	0.8649	0.1351
317.15	0.8585	0.1415
318.65	0.8525	0.1475
319.85	0.8459	0.1541
321.15	0.8393	0.1607

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Circulating water bath, analytical balance, and laser monitoring system. Preweighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and the temperature gradually increased at a rate 0.5 K/20 min (0.2 K/20 min or slower near saturation temperature) until all of the solid solute dissolved. The temperature at which all of the solute dissolved was determined using laser monitoring.

Source and Purity of Chemicals:
(1) <99%, Chemical source not specified, used as received.
(2) <99%, Chemical source not specified, used as received.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±0.0005.

62.6. 2-Nitrobenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Propanone; C_3H_6O; [67-64-1]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
310.8	0.7415	0.2585
341.4	0.6334	0.3666
348.4	0.6068	0.3932
370.8	0.4868	0.5132
375.1	0.4616	0.5384
386.7	0.3745	0.6255
403.1	0.2238	0.7762

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:
(1) Certified Pure, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized twice from aqueous solution. Melting point temperature of purified sample was 420.9 K.
(2) Certified Pure, Merck Chemical Company, was dried over calcium chloride and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_2: ±10% (relative error, estimated by compiler).

62.7. 2-Nitrobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 2-Nitrobenzoic acid; $C_7H_5NO_4$; [552-16-9] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.98 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Baker Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

63. Solubility of 3-Nitrobenzoic Acid in Organic Solvents

63.1. Critical evaluation of experimental solubility data

There have been several published studies[10,54,72,83,99,126,127,180,181] investigating the solubility behavior of 3-nitrobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Charlton *et al.*[10] measured the solubility of 3-nitrobenzoic acid in 17 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 1-hexanol, 2-methyl-1-pentanol, 1-heptanol, 1-octanol, and

1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in three alkyl alkanoates (methyl ethanoate, ethyl ethanoate, and butyl ethanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to revise and update the existing values that the authors had for the Abraham solute descriptors of 3-nitrobenzoic acid. The authors were able to assemble a total of 48 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 3-nitrobenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -1.68$.[176] The McGowan volume of 3-nitrobenzoic acid, $V = 1.1059$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.990$. This left four solute descriptors (S, A, B, and L) still to be determined. The 48 equations were then solved using the Microsoft “SOLVER” program to yield numerical values of the remaining four solute descriptors, $S = 1.180$, $A = 0.730$, $B = 0.520$, and $L = 5.6011$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -8.610$ for the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.072 and 0.094 $\log_{10}$ units, respectively.

After the 3-nitrobenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, methyl ethanoate, ethyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 3-nitrobenzoic acid solubility data. Table 46 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 3-nitrobenzoic acid, x_1, determined by Charlton *et al.*,[10] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1 V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 3-nitrobenzoic acid, $V_{\mathrm{solute}} = 117.7\ \mathrm{cm^3\ mol^{-1}}$, was estimated as the molar volume of benzoic acid ($V_{\mathrm{benzoic\ acid}} = 104.4\ \mathrm{cm^3\ mol^{-1}}$) + molar volume of nitrobenzene ($V_{\mathrm{nitrobenzene}} = 102.7\ \mathrm{cm^3\ mol^{-1}}$) – molar volume of benzene ($V_{\mathrm{benzene}} = 89.40\ \mathrm{cm^3\ mol^{-1}}$). Any errors resulting from the estimation of 3-nitrobenzoic acid's hypothetical subcooled liquid molar volume, V_{solute}, or the ideal molar-volume approximation should have only a very small effect on the calculated c_1 values. 3-Nitrobenzoic acid is not very soluble in many of the solvents considered, and the $x_1 V_{\mathrm{solute}}$ term contributes very little to the molar volume of the saturated solution. Examination of the numerical entries in Table 46 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

TABLE 46. Comparison between observed and calculated molar solubilities of 3-nitrobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp,a}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Methanol	0.568	0.460	0.419
Ethanol	0.408	0.421	0.401
1-Propanol	0.262	0.275	0.281
2-Propanol	0.306	0.288	0.309
1-Butanol	0.184	0.144	0.157
2-Butanol	0.286	0.192	0.183
2-Methyl-1-propanol	0.071	0.093	0.066
2-Methyl-2-propanol	0.339	0.244	0.307
1-Pentanol	0.114	0.153	0.158
2-Pentanol	0.200	0.164	0.155
3-Methyl-1-butanol	0.116	0.078	0.059
1-Hexanol	0.047	0.088	0.081
1-Heptanol	−0.007	0.012	0.042
1-Octanol	−0.026	−0.017	−0.075
1-Decanol	−0.115	−0.093	−0.085
1,1′-Oxybisethane	0.076	−0.139	−0.061
Tetrahydrofuran	0.581	0.632	0.608
1,4-Dioxane	0.322	0.367	0.351
Methyl ethanoate	0.236	−0.002	−0.023
Ethyl ethanoate	0.135	0.015	0.017
Butyl ethanoate	−0.084	−0.155	−0.184

[a]Experimental data were taken from Charlton *et al.*[10]

There have also been a few published papers reporting 3-nitrobenzoic acid solubilities in organic solvents as a function of temperature. Sidgwick and Ewbank[127] measured the solubility of 3-nitrobenzoic acid in benzene. Collett and Lazzell[180] later performed solubility measurements for 3-nitrobenzoic acid in benzene, 1,1′-oxybisethane, trichloromethane, tetrachloromethane and propanone. The internal consistency of the six datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 47, along with the MRD, calculated according to Eq. (24). The largest MRD occurs in the 3-nitrobenzoic acid – tetrachloromethane system, and corresponds to about a 14% error in back-calculating the observed mole fraction solubilities. As noted in the table

TABLE 47. Parameters of the Modified Apelblat equation for describing the solubility of 3-nitrobenzoic acid in various organic solvents

Solvent	A	B	C	MRD (%)
Benzene[a]	−101.165	−2.046	16.864	7.15
Benzene[b]	−103.906	−2.100	17.329	10.34
1,1′-Oxybisethane[b]	−32.134	−0.681	5.310	7.25
Trichloromethane[b]	−71.525	−1.467	11.907	6.19
Tetrachloromethane[b]	−249.472	−4.655	41.634	13.81
Propanone[b]	−28.705	−0.424	4.760	2.68

[a]Calculated from the dataset of Sidgwick and Ewbank.[127]

[b]Calculated from the dataset of Collett and Lazzell.[180] For benzene, the last data point was removed from the regression analysis in order to obtain a reasonable representation. For tetrachloromethane, the first and last data points were removed from the regression analysis in order to obtain a reasonable correlation.

footnote, the first and last data points had to be removed from the regression analysis in order to obtain a reasonable mean relative deviation. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to changes in the liquid phase composition due to solvent evaporation into the vapor phase, and the large range covered by the experimental values, $x_1 = 0.00135$ to $x_1 = 0.833$. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

Jia *et al.*[99] determined the solubility of 3-nitrobenzoic acid in 1-octanol in the temperature range from 293 to 323 K. The calculated curve-fit parameters from the Buchowski λh-model (see Eq. (9)) of $\lambda = 1.866$ and $h = 1274.18$ described the observed solubility data to within a mean relative deviation of 0.7%.

The experimental solubility data for 3-nitrobenzoic acid in organic solvents are in Secs. 63.2–63.9.

63.2. 3-Nitrobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9966	0.00340

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

63.3. 3-Nitrobenzoic acid solubility data in aromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Benzene; C_6H_6; [71-43-2]	[54]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9918	0.00824

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±3% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
306.2	0.991	0.00921
321.2	0.976	0.0238
338.4	0.951	0.0487
362.7	0.830	0.170
378.2	0.632	0.368
394.2	0.354	0.646

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 414.6 K.
(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:

Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Benzene; C_6H_6; [71-43-2]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.7	0.9937	0.00628
323.8	0.9773	0.0227
333.9	0.9664	0.0336
345.0	0.9355	0.0645
353.5	0.8975	0.1025
366.6	0.7755	0.2245
377.4	0.6336	0.3664
382.6	0.5242	0.4758
385.6	0.4670	0.5330
398.0	0.2761	0.7239
408.0	0.1115	0.8885

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:

(1) Purity not given, Synthesized by the authors according to the published method of Holleman [Recl. Trav. Chim. **18**, 267 (1899)], was washed with water, recrystallized from trichloromethane, and recrystallized again from water to give a purified sample having a melting point temperature of 414.6 K.
(2) Thiophene-free, Kahlbaum, was dried over sodium and distilled before use.

Estimated Error:

Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

63.4. 3-Nitrobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.853	0.147

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.862	0.138

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.892	0.108

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.8539	0.1461

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

63.5. 3-Nitrobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.873	0.127

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.8658	0.1342
325.2	0.7867	0.2133
345.1	0.7020	0.2980
355.1	0.6404	0.3596
362.8	0.5820	0.4180
371.6	0.5118	0.4882
386.2	0.3849	0.6151
395.4	0.2802	0.7198
406.2	0.1364	0.8636

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized by the authors according to the published method of Holleman [Recl. Trav. Chim. **18**, 267 (1899)], was washed with water, recrystallized from trichloromethane, and recrystallized again from water to give a purified sample having a melting point temperature of 414.6 K.
(2) U.S.P. grade, Chemical source not given, washed three times with distilled water, dried over calcium chloride, and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_2: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9409	0.0591

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9654	0.0346

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.640	0.360

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.807	0.193

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

63.6. 3-Nitrobenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Trichloromethane; $CHCl_3$; [67-66-3]	[180] A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
320.9	0.9431	0.0569
340.7	0.8836	0.1164
358.5	0.7718	0.2282
373.0	0.6173	0.3827
373.2	0.6139	0.3861
373.7	0.6106	0.3894
379.0	0.5294	0.4706
387.1	0.4168	0.5832
397.5	0.2807	0.7193
405.3	0.1503	0.8497

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized by the authors according to the published method of Holleman [Recl. Trav. Chim. **18**, 267 (1899)], was washed with water, recrystallized from trichloromethane, and recrystallized again from water to give a purified sample having a melting point temperature of 414.6 K.
(2) Certified Pure, Merck Chemical Company, dried over calcium chloride and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_2: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Tetrachloromethane; CCl_4; [56-23-5]	[180] A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
302.6	0.9986	0.00135
368.8	0.9663	0.0337
380.4	0.9048	0.0952
385.5	0.7963	0.2037
389.1	0.6468	0.3532
390.2	0.6035	0.3965
392.5	0.4854	0.5146
398.9	0.3132	0.6862
405.5	0.1670	0.8330

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized by the authors according to the published method of Holleman [Recl. Trav. Chim. **18**, 267 (1899)], was washed with water, recrystallized from trichloromethane, and recrystallized again from water to give a purified sample having a melting point temperature of 414.6 K.
(2) Certified Pure, Merck Chemical Company, dried over calcium chloride and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_2: ±10% (relative error, estimated by compiler).

63.7. 3-Nitrobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Methanol; CH_4O; [67-56-1]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.789	0.211

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Methanol; CH_4O; [67-56-1]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973). [181]I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 3.46 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by the conductance method.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, refluxed over silver oxide, distilled and dehydrated with magnesium.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Ethanol; C_2H_6O; [64-17-5]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.825	0.175

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Ethanol; C_2H_6O; [64-17-5]	[126]P. K. Biswas, S. C. Lahiri, and B. P. Dey, Bull. Chem. Soc. Jpn. **66**, 2785 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
1.6157	0.8952	0.1048

[a]c_1: solubility of the solute expressed in units of mol dm^{-3}.
[b]x_2: mole fraction of component 2 in the saturated solution.
[c]x_1: mole fraction solubility of the solute calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and an ultraviolet/visible spectrophotometer.
Solutions containing excess solute and solvent were allowed to equilibrate at constant temperature for at least 24 h. An aliquot of the saturated solution was removed, filtered, and the absorbance recorded. Solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Puris grade, Fluka Chemicals, recrystallized from aqueous ethanol mixture and dried in an air oven at 390 K. The purified compound was stored in vacuum desiccators.
(2) Absolute, B.C.P.W., Calcutta, India, was distilled twice before use.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±1.0% (relative error, estimated by compiler).
x_1: ±2.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 4.795 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.1809$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Propanol; C_3H_8O; [71-23-8]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.851	0.149

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2-Propanol; C_3H_8O; [67-63-0]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.830	0.170

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.854	0.146

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.812	0.188

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.887	0.113

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.783	0.217

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.857	0.143

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.824	0.176

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Acros Organic, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.890	0.110

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.855	0.145

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.861	0.139

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.866	0.134

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99%, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.864	0.136

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.856	0.144

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[99]Q. Jia, P. Ma, S. Ma, and C. Wang, Chin. J. Chem. Eng. **15**, 710 (2007).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
296.25	0.8259	0.1741
297.25	0.8213	0.1787
299.15	0.8144	0.1856
300.25	0.8063	0.1937
302.90	0.8012	0.1988
303.38	0.7904	0.2094
305.85	0.7806	0.2194
308.45	0.7866	0.2312
311.75	0.7530	0.2470
313.80	0.7379	0.2621
316.25	0.7251	0.2749
317.65	0.7133	0.2867
322.15	0.6945	0.3055

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature circulating bath, stirrer, analytical balance, and laser monitoring system.
Solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent were placed in a stoppered equilibrium vessel, which was connected to a circulating constant-temperature water bath. The solution was stirred and the temperature slowly increased until all of the solid dissolved. Near the dissolution temperature, the temperature was increased at a rate of 0.2 K/20 min. Complete dissolution was determined using a laser monitoring system.

Source and Purity of Chemicals:
(1) 99+%, Chemical source not specified, no purification details were provided.
(2) 99+%, Chemical source not specified, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±1% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.861	0.139

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

63.8. 3-Nitrobenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Propanone; C_3H_6O; [67-64-1]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.2	0.8477	0.1523
301.2	0.7730	0.2270
338.0	0.6168	0.3832
361.2	0.4892	0.5108
377.2	0.3847	0.6153
393.9	0.2317	0.7683

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:
(1) Purity not given, Synthesized by the authors according to the published method of Holleman [Recl. Trav. Chim. **18**, 267 (1899)], was washed with water, recrystallized from trichloromethane, and recrystallized again from water to give a purified sample having a melting point temperature of 414.6 K.
(2) Certified Pure, Merck Chemical Company, was dried over calcium chloride and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_2: ±10% (relative error, estimated by compiler).

63.9. 3-Nitrobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[10]A. K. Charlton, C. R. Daniels, R. M. Wold, E. Pustejovsky, W. E. Acree, Jr., and M. H. Abraham, J. Mol. Liq. **116**, 19 (2005).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9166	0.0834

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 280 nm.

Source and Purity of Chemicals:
(1) 99%, Acros Organics, USA, and also from Aldrich Chemical Company, Milwaukee, WI, USA, was used as received.
(2) 99.7%, anhydrous, Aldrich Chemical Company, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 3-Nitrobenzoic acid; $C_7H_5NO_4$; [121-92-6] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[83]M. K. Chantooni and I. M. Kolthoff, J. Phys. Chem. **77**, 527 (1973).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.78 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) Purity not given, Baker Chemical Company, USA, was recrystallized from either aqueous or aqueous-ethanol solution and dried *in vacuo* at 333 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

64. Solubility of 4-Nitrobenzoic Acid in Organic Solvents

64.1. Critical evaluation of experimental solubility data

There have been several published studies[11,54,63,72,76,126,127,129,130,136,180,181] investigating the solubility behavior of 4-nitrobenzoic acid in organic solvents of varying polarity and hydrogen-bonding capability. Hoover *et al.*[11] measured the solubility of 4-nitrobenzoic acid in 19 alcohols (methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1-pentanol, 2-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 2-methyl-2-butanol, 1-hexanol, 2-methyl-1-pentanol, 4-methyl-2-pentanol, 1-heptanol, 1-octanol, and 1-decanol), in three dialkyl ethers (1,1′-oxybisethane, 2,2′-oxybispropane, and 1,1′-oxybisbutane) and two cyclic ethers (tetrahydrofuran and 1,4-dioxane), in four alkyl alkanoates (methyl ethanoate, ethyl ethanoate, butyl ethanoate, and pentyl ethanoate), and in propylene carbonate at 298 K. Results of the experimental measurements were used to calculate Abraham solute descriptors of 4-nitrobenzoic acid. The authors were able to assemble a total of 51 $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) equations for which experimental partition coefficient data, solubility ratios, Abraham model equation coefficients and aqueous molar solubility were available. The logarithm of the aqueous molar solubility of 4-nitrobenzoic acid is $\log_{10} c_{1,\mathrm{W}} = -2.98$.[72] The McGowan volume of 4-nitrobenzoic acid, $V = 1.1059$, was calculated from the number of chemical bonds in the molecule and the individual atomic group volumes, AV_i, given in Sec. 1.3. The excess molar refraction solute descriptor was estimated as $E = 0.990$. This left four solute descriptors (S, A, B, and L) still to be determined. The 48 equations were then solved using the Microsoft “SOLVER” program to yield numerical values of the remaining four solute descriptors, $S = 1.520$, $A = 0.680$, $B = 0.440$, and $L = 5.7699$, that best described the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values. The computation treated $\log_{10} c_{1,\mathrm{G}}$ as a floating parameter to be determined as part of the regression analyses. The data analyses returned a value of $\log_{10} c_{1,\mathrm{G}} = -9.880$ for the gas-phase solute concentration that made the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) predictions internally consistent. The calculated molecular solute descriptors reproduced the $\log_{10}$ (*SR* or *P*) and $\log_{10}$ (*GSR* or *K*) values to within an average standard deviation of 0.058 and 0.088 $\log_{10}$ units, respectively.

After the 4-nitrobenzoic acid solubility study was published, Abraham model correlations have been developed for 2-pentanol, 3-methyl-1-butanol, methyl ethanoate, and butyl ethanoate, and equation coefficients for a few solvents were updated based on additional experimental data. The new correlations (listed in Tables 1 and 2) will be used in illustrating the ability of the Abraham model to correlate the experimental 4-nitrobenzoic acid solubility data. Table 48 compares the experimental $\log_{10} c_1$ values to calculated values based on Eqs. (20) and (21) of the Abraham model. For comparison purposes, the measured mole fraction solubilities of 4-nitrobenzoic acid, x_1, determined by Hoover *et al.*[11] were converted into molar solubilities by dividing x_1 by the ideal molar volume of the saturated solution (i.e., $c_1^{\mathrm{sat}} = x_1/[x_1V_1 + (1 - x_1)V_{\mathrm{solvent}}]$). The molar volume of the hypothetical subcooled liquid 4-nitrobenzoic acid, $V_{\mathrm{solute}} = 117.7\ \mathrm{cm^3\ mol^{-1}}$, was estimated as the molar volume of benzoic acid ($V_{\mathrm{benzoic\ acid}} = 104.4\ \mathrm{cm^3\ mol^{-1}}$) + molar volume of nitrobenzene ($V_{\mathrm{nitrobenzene}} = 102.7\ \mathrm{cm^3\ mol^{-1}}$) – molar volume of benzene ($V_{\mathrm{benzene}} = 89.40\ \mathrm{cm^3\ mol^{-1}}$). Any errors resulting from the estimation of 4-nitrobenzoic acid’s hypothetical subcooled liquid molar volume, V_{solute}, or the ideal molar-volume approximation should have only a very small effect on the calculated c_1 values. 4-Nitrobenzoic acid is not very soluble in many of the solvents considered, and the x_1V_{solute} term contributes very little to the molar volume of the saturated solution. Examination of the entries in Table 48 reveals that the Abraham model provides a reasonably accurate mathematical description of the observed solubility data, suggesting that there are no obvious outliers in the dataset.

TABLE 48. Comparison between observed and calculated molar solubilities of 4-nitrobenzoic acid based on the Abraham model, Eqs. (20) and (21)

Solvent	$\log_{10} c_1^{\mathrm{exp,a}}$	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (20)	$\log_{10} c_1^{\mathrm{calc}}$; Eq. (21)
Methanol	−0.719	−0.697	−0.632
Ethanol	−0.841	−0.816	−0.769
1-Propanol	−0.975	−0.935	−0.910
2-Propanol	−0.956	−0.930	−0.898
1-Butanol	−1.063	−1.028	−0.993
2-Butanol	−1.017	−0.982	−1.007
2-Methyl-1-propanol	−1.183	−1.163	−1.147
2-Methyl-2-propanol	−0.821	−0.904	−0.879
1-Pentanol	−1.067	−1.108	−1.082
2-Pentanol	−1.086	−1.150	−1.102
3-Methyl-1-butanol	−1.178	−1.207	−1.134
1-Hexanol	−1.076	−1.133	−1.124
1-Heptanol	−1.121	−1.128	−1.158
1-Octanol	−1.209	−1.162	−1.261
1-Decanol	−1.271	−1.344	−1.337
1,1′-Oxybisethane	−0.902	−1.094	−1.008
Tetrahydrofuran	−0.117	−0.195	−0.234
1,4-Dioxane	−0.317	−0.338	−0.326
Methyl ethanoate	−0.837	−0.758	−0.684
Ethyl ethanoate	−0.902	−0.813	−0.795
Butyl ethanoate	−1.119	−0.985	−1.012

[a]Experimental data were taken from Hoover *et al.*[11]

There have also been a few published papers reporting 4-nitrobenzoic acid solubilities in organic solvents as a function of temperature. Sidgwick and Ewbank[127] measured the solubility of 4-nitrobenzoic acid in benzene. Collett and Lazzell[180] later performed solubility measurements for 4-nitrobenzoic acid in benzene, tetrachloromethane, and propanone. The internal consistency of the two of the four datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The limited number of data points in both the tetrachloromethane and propanone datasets was too small to perform a meaningful regression analysis. The values of the equation coefficients (A, B, and C) for the two benzene datasets are given in Table 49, along with the MRD, calculated according to Eq. (24). The largest MRD occurs for the experimental values determined by Sidgwick and Ewbank,[127]

TABLE 49. Parameters of the Modified Apelblat equation for describing the solubility of 4-nitrobenzoic acid in various organic solvents

Solvent	A	B	C	MRD (%)
Benzene[a]	−139.082	2.458	22.363	10.40
Benzene[b]	−128.582	−2.054	20.658	4.92

[a] Calculated from the dataset of Sidgwick and Ewbank.[127]
[b] Calculated from the dataset of Collett and Lazzell.[180] For benzene, the first data point was removed from the regression analysis in order to obtain a reasonable representation.

and corresponds to about a 10.4% error in back-calculating the observed mole fraction solubilities. The large deviation may be due in part to the fact that the solution temperature is above the solvent's normal boiling point temperature, to changes in the liquid phase composition due to solvent evaporation into the vapor phase, and the large range covered by the experimental values, $x_1 = 0.0465$ to $x_1 = 0.682$. It is more difficult to curve-fit experimental solubility data covering large mole fraction ranges.

The experimental solubility data for 4-nitrobenzoic acid in organic solvents are in Secs. 64.2–64.10.

64.2. 4-Nitrobenzoic acid solubility data in saturated hydrocarbons (including cycloalkanes)

Components:	Original Measurements:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[54] C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9999	0.0000118

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±10% (relative error, by compiler).

64.3. 4-Nitrobenzoic acid solubility data in aromatic hydrocarbons

Components:	Original Measurements:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Benzene; C_6H_6; [71-43-2]	[54] C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9998	0.000166

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Reagent grade, Chemical source not specified, refluxed over phosphorous pentoxide for 24 h, and then distilled through a 3 × 80 cm column filled with 0.32-cm glass helices.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±5% (relative error, by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Benzene; C_6H_6; [71-43-2]	[127]N. V. Sidgwick and E. K. Ewbank, J. Chem. Soc. Trans. **119**, 979 (1921).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
437.7	0.953	0.0465
456.6	0.889	0.111
469.7	0.810	0.190
474.8	0.638	0.362
495.2	0.318	0.682

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. Solubility data reported in units of mass percent. Mole fraction values calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. At the higher temperatures, the concentration of solvent in the liquid solution was corrected for the amount of solvent vapor in the bulb. The correction assumed that the vapor pressure of the saturated solution was one half that of the pure solvent at the solution temperature. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:

(1) Purity not given, prepared and purified by the authors using a published synthetic procedure [see J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920) for synthetic details]. Melting point of the purified solute was 515.6 K.

(2) Purity not given, Chemical source not given, thiophene was removed by treatment with sulfuric acid. Sample was further purified by freezing several times.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Benzene; C_6H_6; [71-43-2]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
297.7	0.9998	0.000156
412.1	0.9842	0.0158
442.1	0.9424	0.0576
451.1	0.9022	0.0978
470.4	0.7737	0.2263
479.6	0.6357	0.3643

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:

Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:

(1) Technical grade, Eastman Kodak Chemical Company, Rochester, NY, USA, was dissolved in dilute aqueous sodium hydroxide, precipitated by addition of hydrochloric acid, and then recrystallized twice from aqueous solution. Purified sample had a melting point temperature of 515.6 K.

(2) Thiophene-free, Kahlbaum, was dried over sodium and distilled before use.

Estimated Error:

Temperature: Not given in paper.

x_1: ±10% (relative error, estimated by compiler).

64.4. 4-Nitrobenzoic acid solubility data in esters

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9883	0.01168

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.5%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9876	0.01237

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.9%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9899	0.01007

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.7%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Pentyl ethanoate; $C_7H_{14}O_2$; [628-63-7]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9925	0.007469

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1,2,3-Triacetoxypropane (Triacetin); $C_9H_{14}O_6$; [102-76-1]	W. E. Acree, Jr., unpublished data.
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9848	0.01542

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method: Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with 2-propanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Acros Organics, USA, stored over molecular sieves before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

64.5. 4-Nitrobenzoic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9901	0.009861

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1,1′-Oxybisethane; $C_4H_{10}O$; [60-29-7]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
460.8	0.9463	0.0537
466.8	0.7454	0.2546

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Technical grade, Eastman Kodak Chemical Company, Rochester, NY, USA, was dissolved in dilute aqueous sodium hydroxide, precipitated by addition of hydrochloric acid, and then recrystallized twice from aqueous solution. Purified sample had a melting point temperature of 515.6 K.
(2) U.S.P., Chemical Source not given, was dried over calcium chloride and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_2: ±10% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2,2′-Oxybispropane; $C_6H_{14}O$; [108-20-3]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9964	0.003621

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1,1′-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9972	0.002806

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.3%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1,2-Dimethoxyethane; $C_4H_{10}O_2$; [110-71-4]	[129]S. H. Ghosh and D. K. Hazra, J. Indian Chem. Soc. **65**, 620 (1988).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $c_1 = 0.8324\ \mathrm{mol\,dm^{-3}}$.

Auxiliary Information

Method/Apparatus/Procedure:
Mechanical shaker and a constant-temperature thermostat.
Excess solute and solvent were placed in a bottle and stoppered. The solution was shaken in a mechanical shaker for 24 h at ambient room temperature. The solution was then thermostated at 298 K for 24 h with occasional shaking. An aliquot of the saturated solution was then removed and filtered. The concentration of the dissolved solute was determined by titration with standard caustic soda using phenolphthalein as indicator.

Source and Purity of Chemicals:
(1) G.R., Merck Chemical Company, was recrystallized from aqueous ethanol mixture.
(2) Purum, Fluka, was shaken with ferrous sulfate and then distilled. The distillate was further purified by refluxing for 12 h and then distilling over metallic sodium.

Estimated Error:
Temperature: ±0.01 K.
c_1: ±1.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9361	0.06393

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.9%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables:	**Prepared by:**
T/K = 303.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.929	0.071

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred using a Soxhlet thimble equipped with a one-hole cork stopper and an inverted U-shaped delivery tube to a second ground-glass stoppered flask suspended in the 303 K water bath. Successive portions of the contents were evaporated at room temperature in a tared aluminum foil weighing dish under a bell jar through which a slow stream of dry air was passed. The second flask plus unused saturated solution and the aluminum foil dish plus residue were weighed. The saturation solubility of the solute was calculated from the recorded mass data and molar masses of the solute and solvent.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9580	0.04203

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±2.0% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[63]C. K. Hancock, J. N. Pawloski, and J. P. Idoux, J. Org. Chem. **32**, 1931 (1967).
Variables: T/K = 303.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.950	0.050

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, Soxhlet thimble, conical flask, and analytical balance.
Excess solute and solvent were placed in a conical flask and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Weighed aliquots of saturated solutions were removed and titrated with a standardized sodium hydroxide solution (carbonate free) using a pH meter. The endpoint of the titration was determined by computing the second derivative in the pH versus volume of sodium hydroxide added.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not specified, was recrystallized several times from aqueous-ethanol mixture, and then dried under vacuum over phosphorous pentoxide.
(2) Practical grade, Chemical source not specified, stored over sodium hydroxide pellets for 24 h, and then passed through 2 × 70-cm chromatographic adsorption columns containing activated alumina. After this treatment, the purified solvent was stored over copper in a nitrogen atmosphere.

Estimated Error:
Temperature: ±0.02 K.
x_1: ±1.0% (relative error).

64.6. 4-Nitrobenzoic acid solubility data in haloalkanes, haloalkenes, and haloaromatic hydrocarbons

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
302.6	0.9999	0.000101
439.8	0.9818	0.0182
471.4	0.9337	0.0663

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature. In a few instances near room temperature, the solubility was determined by agitating the solvent in a thermostat with an excess of solute. After equilibrium had been established, an aliquot of the saturated solution was pipetted, weighed, and the amount of dissolved solute determined with a standard solution of titanium (III) chloride.

Source and Purity of Chemicals:
(1) Technical grade, Eastman Kodak Chemical Company, Rochester, NY, USA, was dissolved in dilute aqueous sodium hydroxide, precipitated by addition of hydrochloric acid, and then recrystallized twice from aqueous solution. Purified sample had a melting point temperature of 515.6 K.
(2) Certified Pure, Merck Chemical Company, was dried over calcium chloride and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_1: ±10% (relative error, estimated by compiler).

64.7. 4-Nitrobenzoic acid solubility data in alcohols

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Methanol; CH_4O; [67-56-1]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9921	0.007881

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.8%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Methanol; CH_4O; [67-56-1]	[181]I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.200 mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by the conductance method.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, refluxed over silver oxide, distilled and dehydrated with magnesium.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	Original Measurements:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Ethanol; C_2H_6O; [64-17-5]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9915	0.008544

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) Absolute, Aaper Alcohol and Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	Original Measurements:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Ethanol; C_2H_6O; [64-17-5]	[126]P. K. Biswas, S. C. Lahiri, and B. P. Dey, Bull. Chem. Soc. Jpn. **66**, 2785 (1993).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

c_1[a]	x_2[b]	x_1[c]
0.05445	0.9968	0.00321

[a] c_1: solubility of the solute expressed in units of mol dm^{-3}.
[b] x_2: mole fraction of component 2 in the saturated solution.
[c] x_1: mole fraction solubility of the solute calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
Analytical balance and an ultraviolet/visible spectrophotometer.
Solutions containing excess solute and solvent were allowed to equilibrate at constant temperature for at least 24 h. An aliquot of the saturated solution was removed, filtered, and the absorbance recorded. Solubility was calculated from the measured absorbance.

Source and Purity of Chemicals:
(1) Puris grade, Fluka Chemicals, recrystallized from aqueous ethanol mixture and dried in an air oven at 390 K. The purified compound was stored in a vacuum desiccators.
(2) Absolute, B.C.P.W., Calcutta, India, was distilled twice before use.

Estimated Error:
Temperature: ±0.2 K (estimated by compiler).
c_1: ±1.0% (relative error, estimated by compiler).
x_1: ±2.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Ethanol; C_2H_6O; [64-17-5]	[72]R. Thuaire, Bull. Soc. Chim. Fr. 3815 (1971).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.190 mol/kg of solvent, which corresponds to a mole fraction solubility of $x_1 = 0.00868$.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by a gravimetric method. The saturated solution was evaporated to dryness and the remaining solid residue was weighed. The solubility was calculated from the mass of the solid residue and mass of saturated solution analyzed.

Source and Purity of Chemicals:
(1) Purity not given, Chemical source not given, no purification details were provided.
(2) Purity not given, Chemical source not given, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±4% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Propanol; C_3H_8O; [71-23-8]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9920	0.007990

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Propanol; C_3H_8O; [67-63-0]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9914	0.008550

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Propanol; C_3H_8O; [67-63-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.111 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous solution and dried *in vacuo* at 343 K.
(2) No Purity given, Fisher Scientific, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9920	0.007973

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.8+%, HPLC grade, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Butanol; $C_4H_{10}O$; [78-92-2]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9911	0.008898

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9939	0.006093

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9857	0.01430

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Arco Chemical Company, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.144 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous solution and dried *in vacuo* at 343 K.
(2) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Pentanol; $C_5H_{12}O$; [71-41-0]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9907	0.009317

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Pentanol; $C_5H_{12}O$; [6032-29-7]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9910	0.008967

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Methyl-1-butanol; $C_5H_{12}O$; [137-32-6]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9941	0.005897

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7]
(2) 2-Methyl-2-butanol; $C_5H_{12}O$; [75-85-4]

Original Measurements:
[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9819	0.01814

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7]
(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

Original Measurements:
[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9927	0.007285

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7]
(2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]

Original Measurements:
[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).

Variables:
T/K = 298.15

Prepared by:
W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9895	0.01051

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Hexanol; $C_6H_{14}O$; [111-27-3]	[76]M. K. Chantooni and I. M. Kolthoff, Anal. Chem. **51**, 133 (1979).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.084 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous-ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, was recrystallized from aqueous solution and dried *in vacuo* at 343 K.
(2) Yellow Label, Eastman Kodak Chemical Company, Rochester, NY, USA, shaken with calcium hydride and distilled before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Methyl-1-pentanol; $C_6H_{14}O$; [105-30-6]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9935	0.006460

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 4-Methyl-2-pentanol; $C_6H_{14}O$; [108-11-2]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9915	0.008513

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Heptanol; $C_7H_{16}O$; [111-70-6]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables:	**Prepared by:**
T/K = 298.15	W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9893	0.01071

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9902	0.009758

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9898	0.01022

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Alfa Aesar, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

64.8. 4-Nitrobenzoic acid solubility data in alkoxyalcohols

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Methoxyethanol; $C_3H_8O_2$; [109-86-4]	[129]S. H. Ghosh and D. K. Hazra, J. Indian Chem. Soc. **65**, 620 (1988).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be $c_1 = 0.4884$ mol dm^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Mechanical shaker and a constant-temperature thermostat.
Excess solute and solvent were placed in a bottle and stoppered. The solution was shaken in a mechanical shaker for 24 h at ambient room temperature. The solution was then thermostated at 298 K for 24 h with occasional shaking. An aliquot of the saturated solution was then removed and filtered. The concentration of the dissolved solute was determined by titration with standard caustic soda using phenolphthalein as indicator.

Source and Purity of Chemicals:
(1) G.R., Merck Chemical Company, was recrystallized from aqueous ethanol mixture.
(2) G.R., Merck Chemical Company, was distilled twice before use.

Estimated Error:
Temperature: ±0.01 K.
c_1: ±1.5% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Ethoxyethanol; $C_4H_{10}O_2$; [110-80-5]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9699	0.0301

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Propoxyethanol; $C_5H_{12}O_2$; [2807-30-9]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9753	0.0247

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Isopropoxyethanol; $C_5H_{12}O_2$; [109-59-1]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9719	0.0281

[a]x_2: mole fraction of component 2 in the saturated solution.
[b]x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 2-Butoxyethanol; $C_6H_{14}O_2$; [111-76-2]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9750	0.0250

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99+%, Acros Organics, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 3-Methoxy-1-butanol; $C_5H_{12}O_2$; [2517-43-3]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9739	0.0261

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) 1-Methyl-2-*tert*-butoxyethanol; $C_7H_{16}O_2$; [57018-52-7]	[130]L. M. Grubbs, M. Saifullah, N. E. De La Rosa, S. Ye, S. S. Achi, W. E. Acree, Jr., and M. H. Abraham, Fluid Phase Equilib. **298**, 48 (2010).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9676	0.0324

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99%, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

64.9. 4-Nitrobenzoic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Propanone; C_3H_6O; [67-64-1]	[180]A. R. Collett and C. L. Lazzell, J. Phys. Chem. **34**, 1838 (1930).
Variables: Temperature	**Prepared by:** W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
345.7	0.9626	0.0374
378.5	0.8952	0.1048
420.5	0.7809	0.2191
437.3	0.7122	0.2878

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute. The solubility is given as molal percentage, which, based on the description of 100 times the mole fraction, is taken to be mole percentage.

Auxiliary Information

Method/Apparatus/Procedure:
Preweighed quantities of solute and solvent were placed in bulbs, which were then sealed and heated in a suitable bath. The temperature at which the solid completely dissolved was recorded, and was taken to be the solid-liquid equilibrium temperature.

Source and Purity of Chemicals:
(1) Technical grade, Eastman Kodak Chemical Company, Rochester, NY, USA, was dissolved in dilute aqueous sodium hydroxide, precipitated by addition of hydrochloric acid, and then recrystallized twice from aqueous solution. Purified sample had a melting point temperature of 515.6 K.
(2) Certified Pure, Merck Chemical Company, was dried over calcium chloride and distilled twice before use.

Estimated Error:
Temperature: Not given in paper.
x_2: ±10% (relative error, estimated by compiler).

64.10. 4-Nitrobenzoic acid solubility data in miscellaneous organic solvents

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Propylene carbonate; $C_4H_6O_3$; [108-32-7]	[11]K. R. Hoover, R. Coaxum, E. Pustejovsky, D. M. Stovall, W. E. Acree, Jr., and M. H. Abraham, Phys. Chem. Liq. **42**, 339 (2004).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

x_2[a]	x_1[b]
0.9951	0.004850

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Constant-temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.
Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions were transferred through a coarse filter into tared volumetric flasks, weighed, and diluted with methanol. Concentrations were determined by spectrophotometric measurements at 272 nm.

Source and Purity of Chemicals:
(1) 99+%, Acros Organics, USA, was used as received.
(2) 99.7%, anhydrous, Aldrich Chemical Company, Milwaukee, WI, USA, stored over molecular sieves and distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K.
x_1: ±1.5% (relative error).

Components:	**Original Measurements:**
(1) 4-Nitrobenzoic acid; $C_7H_5NO_4$; [62-23-7] (2) Ethanenitrile; C_2H_3N; [75-05-8]	[136]M. K. Chantooni, Jr. and I. M. Kolthoff, J. Phys. Chem. **78**, 839 (1974).
Variables: T/K = 298.15	**Prepared by:** W. E. Acree, Jr.

Experimental Values

The measured solubility was reported to be 0.041 mol dm^{-3}. The authors did not give the temperature at which the solubility was measured. Based on the experimental description given in an earlier paper [I. M. Kolthoff, J. J. Lingane, and W. Larson, J. Am. Chem. Soc. **60**, 2512 (1938)], the compiler believes the temperature to be 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
Very little experimental details were provided. Solubility was determined by titrating a filtered aliquot of the saturated solution alkalimetrically in an aqueous ethanol mixture using phenolphthalein as the acid-base indicator.

Source and Purity of Chemicals:
(1) White Label, Eastman Kodak Chemical Company, Rochester, NY, USA, recrystallized from aqueous solution and dried *in vacuo* at 343 K.
(2) Purity not given, Chemical source not given, was purified by shaking with saturated potassium hydroxide, followed by activated alumina, and then anhydrous calcium chloride to remove water. Ethanenitrile was further dried over anhydrous magnesium sulfate and then phosphorous pentoxide. The sample was distilled shortly before use.

Estimated Error:
Temperature: ±0.1 K (estimated by compiler).
c_1: ±2% (relative error, estimated by compiler).

65. Solubility of 3-Nitro-1,2-benzenedicarboxylic Acid in Organic Solvents

65.1. Critical evaluation of experimental solubility data

There has been only a single study reporting the solubility of 3-nitro-1,2-benzenedicarboxylic acid in organic solvents. Wang *et al.*[182] used a dynamic method with laser monitoring to determine the solubility of 3-nitro-1,2-benzenedicarboxylic acid in four alkyl alkanoates (ethyl methanoate, methyl ethanoate, ethyl ethanoate, and butyl ethanoate), in two cyclic ethers (tetrahydrofuran and 1,4-dioxane), and in one alkanone (propanone) solvent as a function of temperature. The internal consistency of the seven datasets was assessed by curve-fitting the measured mole fraction solubility data to Eq. (8). The values of the equation coefficients (A, B, and C) are given in Table 50, along with the RMSD, calculated according to Eq. (35). The largest RMSD occurs in the 3-nitro-1,2-benzenedicarboxylic acid – dioxane system, and corresponds to about a 5% error in back-calculating the observed mole fraction solubilities. Results of the mathematical representation analyses indicate that the experimental data for all seven 3-nitro-1,2-benzenedicarboxylic acid – organic solvent systems are internally consistent.

TABLE 50. Parameters of the Modified Apelblat equation for describing the solubility of 3-nitro-1,2-benzenedicarboxylic acid in various organic solvents[a]

Solvent	A	B	C	10^4 RMSD
Ethyl methanoate	−147.71	4843.3	21.02	0.10
Methyl ethanoate	−54.07	1746	7.8873	0.97
Ethyl ethanoate	−103.18	3427.5	15.275	0.42
Butyl ethanoate	148.35	−9015.2	−21.697	0.87
Tetrahydrofuran	−19.492	735.44	2.7106	0.42
1,4-Dioxane	178.46	−9552.9	−26.11	8.71
Propanone	−79.296	2807.6	11.772	0.21

[a] Values of the coefficients and root-mean-square deviations were taken from Wang *et al.*[182]

The experimental solubility data for 3-nitro-1,2-benzenedicarboxylic acid in different organic solvents are in Secs. 65.2–65.4.

65.2. 3-Nitro-1,2-benzenedicarboxylic acid solubility data in esters

Components:	**Original Measurements:**
(1) 3-Nitro-1,2-benzenedicarboxylic acid; $C_8H_5NO_6$; [603-11-2] (2) Ethyl methanoate; $C_3H_6O_2$; [109-94-4]	[182] S. Wang, Q.-S. Li, X. Z. Lin, H. R. Wang, and L. Liu, J. Chem. Eng. Data **52**, 876 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.17	0.9973	0.002679
288.18	0.9971	0.002866
293.21	0.9969	0.003088
298.26	0.9967	0.003346
303.16	0.9964	0.003631
308.19	0.9960	0.003956
313.27	0.9957	0.004329
318.25	0.9953	0.004729
323.29	0.9948	0.005173

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, circulating water temperature controller, stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and small quantities of solid solute were added until the saturation point was reached. The saturation point was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.4%, Zhe Jiang Lianhe Chemical Technology Company, Ltd., China, no purification details were provided.
(2) Analytical Reagent grade, Shanghai Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitro-1,2-benzenedicarboxylic acid; $C_8H_5NO_6$; [603-11-2] (2) Methyl ethanoate; $C_3H_6O_2$; [79-20-9]	[182] S. Wang, Q.-S. Li, X. Z. Lin, H. R. Wang, and L. Liu, J. Chem. Eng. Data **52**, 876 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.17	0.9666	0.03344
283.26	0.9657	0.03431
288.27	0.9646	0.03535
293.21	0.9635	0.03652
298.24	0.9622	0.03783
303.16	0.9608	0.03922
308.22	0.9593	0.04071
313.28	0.9578	0.04224
318.17	0.9563	0.04373
323.19	0.9548	0.04524

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, circulating water temperature controller, stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and small quantities of solid solute were added until the saturation point was reached. The saturation point was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.4%, Zhe Jiang Lianhe Chemical Technology Company, Ltd., China, no purification details were provided.
(2) Analytical Reagent grade, Shanghai Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitro-1,2-benzenedicarboxylic acid; $C_8H_5NO_6$; [603-11-2] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	[182]S. Wang, Q.-S. Li, X. Z. Lin, H. R. Wang, and L. Liu, J. Chem. Eng. Data **52**, 876 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.20	0.9921	0.007926
288.26	0.9915	0.008467
293.28	0.9910	0.009015
298.19	0.9904	0.009577
303.21	0.9898	0.01019
308.30	0.9891	0.01088
313.16	0.9884	0.01160
318.22	0.9876	0.01244
323.16	0.9866	0.01337
328.23	0.9856	0.01443
333.17	0.9844	0.01561

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, circulating water temperature controller, stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and small quantities of solid solute were added until the saturation point was reached. The saturation point was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.4%, Zhe Jiang Lianhe Chemical Technology Company, Ltd., China, no purification details were provided.
(2) Analytical Reagent grade, Shanghai Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitro-1,2-benzenedicarboxylic acid; $C_8H_5NO_6$; [603-11-2] (2) Butyl ethanoate; $C_6H_{12}O_2$; [123-86-4]	[182]S. Wang, Q.-S. Li, X. Z. Lin, H. R. Wang, and L. Liu, J. Chem. Eng. Data **52**, 876 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
283.18	0.9976	0.002433
288.16	0.9970	0.002970
293.21	0.9965	0.003532
298.19	0.9959	0.004103
303.22	0.9953	0.004698
308.26	0.9947	0.005312
313.27	0.9941	0.005939
318.18	0.9936	0.006570
323.22	0.9928	0.007236
328.24	0.9921	0.007917
333.19	0.9914	0.008605
338.28	0.9907	0.009330
343.25	0.9899	0.01006
348.24	0.9892	0.01080
353.26	0.9884	0.01157

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, circulating water temperature controller, stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and small quantities of solid solute were added until the saturation point was reached. The saturation point was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.4%, Zhe Jiang Lianhe Chemical Technology Company, Ltd., China, no purification details were provided.
(2) Analytical Reagent grade, Shanghai Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

65.3. 3-Nitro-1,2-benzenedicarboxylic acid solubility data in ethers

Components:	**Original Measurements:**
(1) 3-Nitro-1,2-benzenedicarboxylic acid; $C_8H_5NO_6$; [603-11-2] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	[182]S. Wang, Q.-S. Li, X. Z. Lin, H. R. Wang, and L. Liu, J. Chem. Eng. Data **52**, 876 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.28	0.7966	0.2034
283.17	0.7962	0.2038
288.16	0.7957	0.2043
293.21	0.7950	0.2050
298.29	0.7943	0.2057
303.28	0.7934	0.2066
308.19	0.7924	0.2076
313.23	0.7912	0.2088
318.24	0.7900	0.2100
323.16	0.7886	0.2114
328.19	0.7871	0.2129
333.17	0.7855	0.2145

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, circulating water temperature controller, stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and small quantities of solid solute were added until the saturation point was reached. The saturation point was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.4%, Zhe Jiang Lianhe Chemical Technology Company, Ltd., China, no purification details were provided.
(2) Analytical Reagent grade, Shanghai Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

Components:	**Original Measurements:**
(1) 3-Nitro-1,2-benzenedicarboxylic acid; $C_8H_5NO_6$; [603-11-2] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[182]S. Wang, Q.-S. Li, X. Z. Lin, H. R. Wang, and L. Liu, J. Chem. Eng. Data **52**, 876 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
288.17	0.9242	0.07583
293.28	0.9132	0.08682
298.31	0.9029	0.09705
303.29	0.8934	0.1066
308.26	0.8844	0.1156
313.20	0.8760	0.1240
318.21	0.8681	0.1319
323.29	0.8607	0.1393
328.19	0.8541	0.1459
333.18	0.8479	0.1521
338.22	0.8422	0.1578
343.16	0.8373	0.1627
348,23	0.8327	0.1673
353.32	0.8288	0.1712

[a] x_2: mole fraction of component 2 in the saturated solution.
[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium jacketed glass vessel, circulating water temperature controller, stirrer, analytical balance, laser monitoring system.
Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and small quantities of solid solute were added until the saturation point was reached. The saturation point was determined using laser monitoring.

Source and Purity of Chemicals:
(1) 99.4%, Zhe Jiang Lianhe Chemical Technology Company, Ltd., China, no purification details were provided.
(2) Analytical Reagent grade, Shanghai Chemical Reagent Company, China, no purification details were provided.

Estimated Error:
Temperature: ±0.05 K.
x_1: ±3% (relative error, estimated by compiler).

65.4. 3-Nitro-1,2-benzenedicarboxylic acid solubility data in ketones

Components:	**Original Measurements:**
(1) 3-Nitro-1,2-benzenedicarboxylic acid; $C_8H_5NO_6$; [603-11-2] (2) Propanone; C_3H_6O; [67-64-1]	[182]S. Wang, Q.-S. Li, X. Z. Lin, H. R. Wang, and L. Liu, J. Chem. Eng. Data **52**, 876 (2007).
Variables:	**Prepared by:**
Temperature	W. E. Acree, Jr.

Experimental Values

T/K	x_2[a]	x_1[b]
278.16	0.9475	0.05249
283.18	0.9459	0.05414
288.27	0.9440	0.05604
293.33	0.4918	0.05815
298.24	0.9396	0.06041
303.19	0.9371	0.06290
308.32	0.9343	0.06570
313.16	0.9314	0.06855
318.20	0.9283	0.07173

[a] x_2: mole fraction of component 2 in the saturated solution.

[b] x_1: mole fraction solubility of the solute.

Auxiliary Information

Method/Apparatus/Procedure:

Equilibrium jacketed glass vessel, circulating water temperature controller, stirrer, analytical balance, laser monitoring system.

Experimental solubilities were determined by a dynamic method. Pre-weighed amounts of solute and solvent and were placed in an equilibrium vessel, which was connected to a circulating water bath. The solution was stirred and small quantities of solid solute were added until the saturation point was reached. The saturation point was determined using laser monitoring.

Source and Purity of Chemicals:

(1) 99.4%, Zhe Jiang Lianhe Chemical Technology Company, Ltd., China, no purification details were provided.

(2) Analytical Reagent grade, Shanghai Chemical Reagent Company, China, no purification details were provided.

Estimated Error:

Temperature: ±0.05 K.

x_1: ±3% (relative error, estimated by compiler).

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