IUPAC-NIST Solubility Data Series. 90. Hydroxybenzoic Acid Derivatives in Binary and Ternary Systems. Part II. Hydroxybenzoic Acids, Hydroxybenzoates, and Hydroxybenzoic Acid Salts in Nonaqueous Systems

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The solid-liquid solubility data for well defined nonaqueous binary and ternary systems are reviewed. One component includes hydroxybenzoic acid, hydroxybenzoate, and hydroxybenzoic acid salt, and another component includes a variety of organic compounds (hydrocarbons, alcohols, halogenated hydrocarbons, carboxylic acids, esters, *et al.*) and carbon dioxide. The ternary systems include mixtures of organic substances of various classes and carbon dioxide. The total number of compilation sheets is 270 for six types of system. Almost all data are expressed as mass percent and mole fraction as well as the originally reported units, while some data are expressed as molar concentration. Critical evaluation was carried out for the binary nonaqueous systems of 2-, 3-, and 4-hydroxybenzoic acids and hydroxybenzoates (methylparaben, ethylparaben, propylparaben, and butylparaben) in alcohols, 1-heptane, and benzene. © *2011 American Institute of Physics*. [doi:10.1063/1.3569816]

Key words: hydroxybenzoic acid; hydroxybenzoic acid salt; nonaqueous systems; paraben; salicylic acid; solubility.

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1. Preface

1.1. Scope of the volume

We have reported the solubilities of hydroxybenzoic acid derivatives in aqueous systems as Part 1 of this volume.[1] This Part 2 reviews experimentally determined solubility data of the hydroxybenzoic acid derivatives for well defined nonaqueous binary and ternary systems of organic compounds. The solutes are as follows: Hydroxybenzoic acid corresponds to 2-, 3-, and 4-hydroxbenzoic acids. 4-Hydroxybenzoic acid alkyl ester (paraben) corresponds to methyl-, ethyl-, propyl-, butyl-, hexyl-, heptyl-, octyl-, decyl-, methylpropyl-, pentyl-, and benzyl esters. Monohy-

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droxybenzoic acid salts correspond to sodium, silver, and ammonium salts. All of the solutes are in the solid state at room temperature.

As another component, a variety of organic solvents (alcohols, halogenated hydrocarbons, carboxylic acids, amides, esters, etc.) were examined, along with supercritical carbon dioxide. This volume includes solid-liquid equilibrium of nonaqueous binary and ternary systems, and the goal of the search of Part 2 is to include all published data for nonaqueous systems designated in the title. The list of solutes included is shown in Table 1.

Hydroxybenzoic acids and the related compounds are important substances closely related to daily life, as described in the previous paper.[1] Recently, hydroxybenzoates (parabens) have been widely used as preservatives in the cosmetic, pharmaceutical, and food industries. Their solubilities in nonaqueous solutions as well as in aqueous solutions are important from the viewpoint of their solution states in micellar solutions and the partition coefficients between water and oil phases, as described by Goto.[2–8]

The solubility data for six classes of systems were found by an exhaustive search of the chemical literature published prior to 2001, as shown in Table 1. From these, 270 compilation sheets were prepared. Most compilations present the solubility data for one system as reported in one publication. They are the result of an exhaustive search of the chemical literature using Chemical Abstracts.

TABLE 1. List of compiled sheets for solutes in nonaqueous binary and ternary systems

	Binary system	Ternary system
Hydroxybenzoic acid (HA)	136	14
Hydroxybenzoic acid ester (HAE)	112	2
Hydroxybenzoic acid salt (HAS)	6	0

In some original sources, solubility data were reported as incidental or ancillary information to other studies. If, for this or other reasons, details concerning experimental methods, source and purity of materials, or estimated errors were brief or absent, correspondingly short entries appear in the compilations, sometime with the note “No further details were reported” or “Not stated” or “Nothing specified.”

For convenience of comparison of experimental data, the compilers and evaluators of this volume, as far as possible, expressed all initial results in mass percent and mole fraction as well as in units reported in the original source. Conversions, where they were made, are clearly attributed to the compiler. Some units require numerical data for the density of pure components and/or the mixtures. Definitions of mass percent and mole fraction as well as their relation to other units of solubility are given in the Introduction to the Solubility Data Series.[9]

1.2. Experimental methods

Most solubility measurements of binary and ternary systems containing each solute have been made from 284.2 to 486.2 K at atmospheric pressure. Samples of liquid phases at equilibrium are analyzed by various methods. Table 2 shows the list of various methods for the measurement of the solubilities. The solubility measurements of hydroxybenzoic acids for binary and ternary systems are mainly carried out by UV spectroscopy, titration, gravimetry, and synthetic method. The basic approach to solubility measurement of hydroxybenzoates for binary and ternary systems is UV spectroscopy, but gravimetry is used in limited systems.

TABLE 2. Analytical methods of solutes in nonaqueous systems

	Binary system			Ternary system			
Method	HA[a]	HAE[b]	HAS[c]	HA	HAE	HAS	Total number[d]
Spectroscopy	46	118(40)	0	0	2	0	166
Titration	22	0	0	5	0	0	27
Gravimetry	29	56(40)	1	9	0	0	95
Synthetic method	11	0	0	0	0	0	11
Other methods[e]	3	1	3	0	0	0	7

[a] HA: Hydroxybenzoic acid.

[b] HAE: Hydroxybenzoic acid ester.

[c] HAS: Hydroxybenzoic acid salt.

[d] The total number of sheets does not correspond with the sum of the different methods because some sheets contain plural analytical methods and some sheets for references whose methods are not described clearly are not counted.

[e] Other methods include thermometry, and measurement of radioisotopes, potential difference, and vapor pressure.

System pressure at the solution temperature is seldom reported because it is assumed that the effect of pressure is minor. With the solvent, a correction was made at higher temperatures for the amount present as vapor in the bulb, and carbon dioxide was also affected by the pressure. Sources of error in these methods include gravitational effects and impurities in materials whose solubilities are determined.

1.3. Procedure used in critical evaluation

Data are recommended if the results of independent groups are in good agreement and the evaluators have no doubt of the adequacy of the experimental and computational procedures used. Data determined by an inadequate or ill-defined method are rejected.

Where two or more reliable compilations were found for a system, a critical evaluation was carried out. This was possible for 36 systems of hydroxybenzoic acids and parabens (methyl-, ethyl-, propyl-, and butylparabens) in binary systems of alcohols, alkane and benzene, as shown in Table 3.

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TABLE 3. List of evaluation sheets for solutes in binary systems of various solvents. ○: evaluated, —: not evaluated

	Solute						
	Hydroxybenzoic Acid (HA)			Hydroxybenzoic Acid Ester[a]			
Organic solvent	2HA	3HA	4HA	MP	EP	PP	BP
Methanol	—	—	—	○	○	○	○
Ethanol	○	○	○	○	○	○	○
1-Propanol	—	—	—	○	○	○	○
1-Butanol	○	—	○	○	○	○	○
1-Hexanol	—	—	—	○	○	○	○
1-Octanol	—	—	—	—	○	○	○
1-Decanol	—	—	—	○	○	○	○
1-Heptane	○	—	—	—	—	—	—
Benzene	○	○	○	—	—	—	—

[a] MP: methylparaben; EP: ethylparaben; PP: propylparaben; BP: butylparaben.

The data for the solubility of the hydroxybenzoic acids and the parabens in organic solvents were treated as a function of absolute temperature. Data for the solubility of the hydroxybenzoic acids and the parabens were fitted to Eq. (1) or (2),[10–12]

$$\ln x_1 = A/T + B \ln T + C, \tag{1}$$

$$\ln x_1 = A/T + C. \tag{2}$$

The equation parameters statistically calculated by the least squares method are presented in the critical evaluations. The solubilities calculated by the proposed equations are presented in the tables; these values are recommended.

A complete guide to the preparation and use of compilations and evaluations for the *IUPAC-NIST Solubility Data Series* can be found in the articles[9] jointly published by IUPAC and NIST. These procedures were applied to all the data sources[2–8,13–45] compiled here.

Of particular interest for the present volume are the uncommon use of the symbols γ for mass concentration and φ for volume fraction. These symbols, defined in Ref. 9, are often found in the pharmaceutical literature, particularly in the older literature.

2. Hydroxybenzoic Acids, Parabens, and Hydroxybenzoic Acid Salts in Binary Nonaqueous Systems

2.1. Hydroxybenzoic acid–organic compound systems

2.1.1. Critical evaluation of the solubility of hydroxybenzoic acids in alkanes

2.1.1.1. Salicylic acid

Components:	**Evaluators:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) *n*-Heptane (heptane); C_7H_{16}; [142-82-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 4. Summary of experimental solubility data of salicylic acid in heptane

T/K	$100m_1$/mol kg^{-1}	$100w_1$	$100x_1$	Analytical method	Reference
298.2	0.33		0.048	Spectroscopy	13
365.4		2.09	1.52[a]	Synthetic method	14
385.6		5.37	3.95[a]	Synthetic method	14
397.9		10.25	7.651[a]	Synthetic method	14
407.5		20.15	1.55[a]	Synthetic method	14
415.2		41.6	3.41[a]	Synthetic method	14
418.7		60.2	5.23[a]	Synthetic method	14
422.7		81.4	7.60[a]	Synthetic method	14

[a] The mole-fraction solubilities were calculated based on w_1.

Solubilities of salicylic acid in heptane were reported in two publications. The measurement was carried out from 298.2 to 422.7 K. The solubilities of salicylic acid in heptane are shown in Table 4, in which molality, mass percent, and mole fraction are expressed as units. The measurement was carried out by the synthetic method and spectroscopy, as shown in Table 4.

Data for the solubility of salicylic acid in heptane expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3. The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 1, but they deviated from Eq. (2). The equation parameters were derived by multiple regression analysis using SPSS based on Eq. (1), with the following results:

Multiple correlation coefficient: 0.996

Sample size: 8 data points

p-value (F test): 0.000

Constants: $A = 24560 \pm 5865$, $B = 89.93 \pm 16.62$, $C = -602.3 \pm 114.3$

White circles in Fig. 1 represent the observed data and the black line corresponds to calculated values according to Eq. (1). ($\ln x_1 = 24560/T + 89.93 \ln T - 602.3$) The observed data fit closely with the calculated values in the range of 298.2–422.7 K, with the multiple correlation coefficient of

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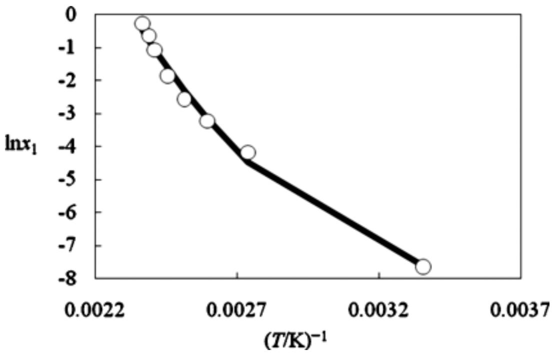

FIG. 1. Fitting curve of Eq. (1) and the observed data for salicylic acid in heptane.

0.996, as shown in Fig. 1. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 5 shows the observed data in the range of 298.2–422.7 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 5. Observed data and recommended values calculated according to Eq. (1) for salicylic acid in heptane

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	0.048	0.0497
365.4	1.52	1.14
385.6	3.95	4.25
397.9	7.651	9.99
407.5	15.5	19.9
415.2	34.1	35.1
418.7	52.3	45.5
422.7	76	61.5

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) *n*-Heptane (heptane); C_7H_{16}; [142-82-5]	[14]N.V. Sidgwick and E.K. Ewbank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°\mathrm{C}=92.2–149.5$	A. Goto and H. Miyamoto

Solubility of salicylic acid in *n*-heptane

Temperature	Solubility	
$t/°\mathrm{C}$	w_1	$100x_1$ (compiler)
92.2	2.09	1.52
112.4	5.37	3.95
124.7	10.25	7.651
134.3	20.15	15.5
142.0	41.6	34.1
145.5	60.2	52.3
149.5	81.4	76.0

Auxiliary Information

Methods/Apparatus/Procedure:

The solubility was determined synthetically. Weighed quantities of the acid and the solvent were enclosed in bulbs, which were then sealed and heated in a suitable bath. With the solvent, a correction was made at higher temperatures for the amount present as vapor in the bulb; for this purpose the vapor pressure of the saturated solution was assumed to be half that of the pure solvent at the same temperature. The thermometers had been compared with a standard instrument, and all readings were corrected.

Source and Purity of Materials:

The preparation and the purification of salicylic acid were described in [J. Walker and J.K Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of the purified acid was 159.0 °C.

n-Heptane was a specimen from *Pinus sabiniana*, which had been purified by treatment with sulfuric and nitric acids, and distillation [T.E. Thorpe, J. Chem. Soc. **35**, 296 (1879)].

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) *n*-Heptane (heptane); C_7H_{16}; [142-82-5]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and H. Miyamoto

Solubility of salicylic acid in *n*-heptane at 25 °C

Solubility	
10^4x_1	$10^3m_1/\mathrm{mol\,kg^{-1}}$
4.8	3.3

Auxiliary Information

Methods/Apparatus/Procedure:

An amount of solid at least five times in excess of its solubility was allowed to equilibrate with the solvent in a stoppered and sealed volumetric flask, which was continuously shaken on a wrist-action shaker in a thermostated bath for at least 24 h. An aliquot of the saturated solution was pipetted out and distilled accurately from 10 to 100 times in chloroform. The concentration of salicylic acid was determined by the UV spectrometric method.

Source and Purity of Materials:

n-Heptane of reagent grade was purified by passing the solvent through a column of silica gel followed by distillation from sodium under reduced pressure.

Salicylic acid was recrystallized from hot water.

Estimated Errors:

Nothing specified.

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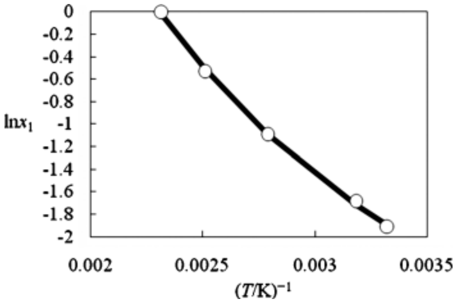

FIG. 2. Fitting curve of Eq. (1) and the observed data for salicylic acid in ethanol.

2.1.2. Critical evaluation of the solubility of hydroxybenzoic acids in alcohols

2.1.2.1. Salicylic acid

Components:	**Evaluators:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 6. Summary of experimental solubility data of salicylic acid in ethanol

T/K	$c_1/\text{mol dm}^{-3}$	$100w_1$	$100x_1$	Analytical method	Reference
293.2	2.041			Gravimetry	15
301.2			14.79	Titration($Ba(OH)_2$)	16
303.8	2.76			Titration(NaOH)	17
314.2		18.6	18.6[a]	Synthetic method	14
358.4		60.4	33.7[a]	Synthetic method	14
398.4		81.2	59.0[a]	Synthetic method	14
432.2		100.0	100.0[a]	Synthetic method	14

[a] The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 4

The range of temperature: $T/\text{K}=293.2-432.2$

The units: mass percent, mole fraction, and mol dm^{-3}

Analytical methods: gravimetry, synthetic method, and titration

Data for the solubility of salicylic acid in ethanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 6). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 2, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

Multiple correlation coefficient: 1.000

Sample size: 5 data points

p-value (F test): 0.001

Constants: $A=2292\pm 839$, $B=11.58\pm 2.35$, $C=-75.60\pm 16.18$

White circles in Fig. 2 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=2292/T+11.58\ln T-75.60$). The observed data fit closely with the calculated values in the range of 298.2–432.2 K, with the multiple correlation coefficient of 1.000, as shown in Fig. 2. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 7 shows the observed data in the range of 298.2–432.2 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 7. Observed data and recommended values calculated according to Eq. (1) for salicylic acid in ethanol

T/K	$100x_1$(obs)	$100x_1$(rec)
301.2	14.79	15.1
314.2	18.6	18.0
358.4	33.7	33.6
398.4	59.0	60.2
432.2	100	98.5

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[14] S.V. Sidgwick and E.K. Embank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°\text{C}=41.0-159.0$	A. Goto and H. Miyamoto

Solubility of salicylic acid in ethanol

Temperature		Solubility
$t/°\text{C}$	$100w_1$	$100x_1$ (compiler)
159.0	100.0	100.0
125.2	81.2	59.0
85.2	60.4	33.7
41.0	40.6	18.6

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and purification methods were described in [J. Walker and J.K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of salicylic acid was 159.0 °C.

Ethanol was distilled over calcium oxide, and the purity determined from the density was 99.0%.

Estimated Errors:

Nothing specified.

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Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
$t/°C=28$	A. Goto and H. Miyamoto

The solubility of salicylic acid in ethanol at 28 °C was reported as $x_1=0.1479$.

Auxiliary Information

Methods/Apparatus/Procedure:

Salicylic acid was saturated in 100 ml of ethanol in a series of flasks, which were kept revolving on a wheel in an air thermostat at 28 °C for 48 h. In order to avoid any error due to the absorption of the solute by the filter paper, a fresh saturated solution was filtered through it before the solution used for the estimation of the acid was passed through. A suitable amount of the filtrate was titrated against barium hydroxide solution using phenolphthalein as an indicator. The stock solution of barium hydroxide was titrated against a standard solution of succinic acid.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

Ethanol was purified by distillation.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results, the precision being less than 0.5%.

Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
$t/°C=20.0$	P. Scharlin

Solubility of salicylic acid in ethanol at 20 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
281.9	2.041

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The solubility apparatus consisted of a 150 ml vessel equipped with a mechanical stirrer and a side tube which connected the vessel to a vacuum filtration system. During the measurements, the apparatus was immersed in a water bath of constant temperature. A known mass of the compound to be studied was introduced into the solubility vessel. The mass varied between 2 and 10 g depending on the expected solubility of the compound. About 20 ml of solvent was added, the apparatus was closed tightly with rubber stoppers and immersed in a water bath so that only the upper part of the solubility vessel stayed above water. Stirring was initiated and the compound allowed to dissolve during 30 min. The solution was vacuum filtered through a stinter and a known volume of filtered solution was transferred to a constant-mass evaporating dish. The solvent was carefully evaporated over a steam bath and the dish was placed in a drying oven. The temperature of the oven did not exceed 100 °C. The dish was allowed to cool to room temperature in a desiccator and weighed. The solubility was calculated as grams per 100 ml of solution.

Source and Purity of Materials:

Salicylic acid was obtained from Shuchardt, DAB6.

Ethanol: source and purity not given; relative density $d=0.789$ (20 °C/4 °C).

Estimated Errors:

Nothing specified. According to the author, the values given are the mean of three independent determinations.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
$t/°C=30.6$	A. Goto, R. Goto, and H. Miyamoto

Solubility of salicylic acid in ethanol at 30.6 °C

	Solubility[a]	
Dielectric constant of solvent	$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
20.7	381	2.76

[a]In the original paper, the solubility was given as milligrams per milliliter of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The solubility of salicylic acid was determined in pure solvent using 15 ml screw-capped vials fitted with Teflon liners. The vials were attached to a rotating wheel in a water bath maintained at 30.6 °C. Equilibration time of 24 h was sufficient. Samples were withdrawn from the reaction vials using a pipet fitted with a glass wool filtering plug. The solubility of salicylic acid was determined by base titration using freshly prepared 0.1 mol dm^{-3} NaOH solution as titrant and phenolphthalein as an indicator. The dielectric constant of the ethanol were measured by a resonance method at 25 °C.

Source and Purity of Materials:

Ethanol was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]

(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan
Rensuke Goto, University of Shizuoka, Shizuoka, Japan
Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 8. Summary of experimental solubility data of salicylic acid in 1-butanol

T/K	$c_1/\mathrm{mol\ dm^{-3}}$	$100w_1$	$100x_1$	Analytical method	Reference
297.2		24.36	14.75[a]	Synthetic method	14
298.15			16.46	Spectroscopy	18
301.2			15.88	Titration(Ba(OH)$_2$)	16
303.8	1.82			Titration(NaOH)	17
311.2		28.88	17.89[a]	Synthetic method	14
358.8		48.9	33.9[a]	Synthetic method	14
394.8		79.2	67.1[a]	Synthetic method	14

[a] The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 4

The range of temperature: $T/\mathrm{K}=297.2-394.8$

The units: mass percent, mole fraction, and mol dm^{-3}

Analytical methods: synthetic method, spectroscopy, and titration

Data for the solubility of salicylic acid in 1-butanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 8). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 3, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

Multiple correlation coefficient: 0.998

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=6769\pm1877$, $B=24.96\pm5.54$, $C=-166.8\pm37.8$

White circles in Fig. 3 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=6769/T+24.96\ln T-166.8$). The observed data fit closely with the calculated values in the range of 297.2–394.8 K, with the multiple correlation coefficient of 0.998, as shown in Fig. 3. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

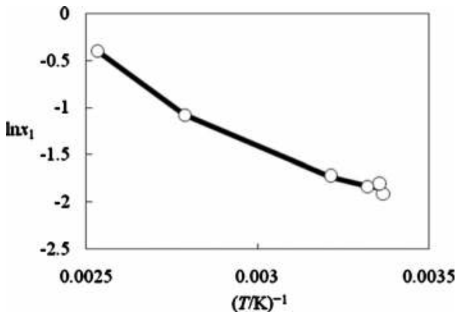

FIG. 3. Fitting curve of Eq. (1) and the observed data for salicylic acid in 1-butanol.

Table 9 shows the observed data in the range of 297.2–394.8 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 9. Observed data and recommended values calculated according to Eq. (1) for salicylic acid in 1-butanol

T/K	$100x_1$(obs)	$100x_1$(rec)
297.2	14.75	15.5
298.15	16.46	15.6
301.2	15.88	16.0
311.2	17.89	17.6
358.8	33.9	34.3
394.8	67.1	66.7

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]

(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:

[14] S.V. Sidgwick and E.K. Embank, J. Chem. Soc. **1921**, 979.

Variables:

$t/°\mathrm{C}=24.0-121.6$

Prepared by:

A. Goto and H. Miyamoto

Solubility of salicylic acid in 1-butanol

Temperature	Solubility	
$t/°\mathrm{C}$	$100w_1$	$100x_1$ (compiler)
121.6	79.2	67.1
85.6	48.9	33.9
38.0	28.88	17.89
24.0	24.36	14.75

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and purification methods were described in [J. Walker and J.K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of salicylic acid was 159.0 °C.

1-Butanol was repeatedly fractionated, and distilled within 0.1 °C.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
$t/°C=28$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 1-butanol at 28 °C was reported as $x_1=0.1588$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

1-Butanol was purified by distillation.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results, the precision being less than 0.5%.

Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
$t/°C=30.6$	A. Goto and H. Miyamoto

Solubility of salicylic acid in 1-butanol at 30.6 °C

Dielectric constant of solvent	Solubility[a] $\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
17.1	251	1.82

[a]In the original paper, the solubility was given as milligrams per milliliter of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvents were purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[18]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:**
$T/K=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 1-butanol at 298.15 K was reported as $x_1=0.1646$.

Auxiliary Information

Methods/Apparatus/Procedure:

Excess solute and solvent were placed in amber glass bottles and allowed to equilibrate in a constant-temperature water bath at 25.0 °C for at least 3 days (often longer). Attainment of equilibrium was verified both by repetitive measurements after several additional days and by approaching equilibrium from supersaturation. Aliquots of saturated salicylic acid solutions were transferred through a coarse filter into a tared volumetric flask to determine the amount of sample and diluted quantitatively with methanol for spectrophotometric analysis. Mole-fraction solubilities were computed from (mass / mass) solubility fraction using the molar masses of the solute and solvent.

Source and Purity of Materials:

Salicylic acid (Aldrich 99+%, ACS Reagent Grade) was dried in an oven for several hours at 80 °C and used without further purification. The purity of salicylic acid was 99.86±0.12 mass %, as determined by five volumetric titrations using a freshly standardized sodium hydroxide titrant and phenolphthalein indicator.

1-Butanol (Aldrich, HPLC, 99.8+%) was stored over molecular sieves before use. Gas chromatographic analysis showed solvent purities to be 99.7 mole % or better.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

2.1.2.2. 3-Hydroxybenzoic acid

Components:	**Evaluators:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Ethyl alcohol (ethanol) C_7H_6O; [64-17-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

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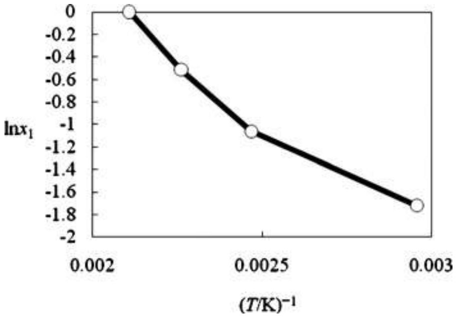

FIG. 4. Fitting curve of Eq. (1) and the observed data for 3-hydroxybenzoic acid in ethanol.

Critical Evaluation

TABLE 10. Summary of experimental solubility data of 3-hydroxybenzoic acid in ethanol

T/K	c_1/mol dm^{-3}	$100w_1$	$100x_1$	Analytical method	Reference
293.2	1.632			Gravimetry	14
338.2		39.6	17.9[a]	Synthetic method	15
405.2		61.3	34.6[a]	Synthetic method	15
442.2		81.7	59.8[a]	Synthetic method	15
474.5		100.0	100.0[a]	Synthetic method	15

[a] The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/\mathrm{K}=293.2-474.5$

The units: mass percent, mole fraction, and mol dm^{-3}

Analytical methods: synthetic method and gravimetry

Data for the solubility of 3-hydroxybenzoic acid in ethanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 10). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 4, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

Multiple correlation coefficient: 1.000

Sample size: 4 data points

p-value (F test): 0.007

Constants: $A=7204\pm281$, $B=23.16\pm0.71$, $C=-157.9\pm5.0$

White circles in Fig. 4 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=7204/T+23.16\ln T-157.9$). The observed data fit closely with the calculated values in the range of 338.2–474.5 K, with the multiple correlation coefficient of 1.000, as shown in Fig. 4. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 11 shows the observed data in the range of 338.2–474.5 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 11. Observed data and recommended values calculated according to Eq. (1) for 3-hydroxybenzoic acid in ethanol

T/K	$100x_1$(obs)	$100x_1$(rec)
338.2	17.9	17.9
405.2	34.6	34.8
442.2	59.8	59.5
474.5	100	100

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[14] S.V. Sidgwick and E.K. Embank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°\mathrm{C}=65.0-201.3$	A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in ethanol

Temperature	Solubility	
t/°C	$100w_1$	$100x_1$ (compiler)
201.3	100.0	100.0
169.0	81.7	59.8
132.0	61.3	34.6
65.0	39.6	17.9

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and purification methods were described in [J. Walker and J.K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of 3-hydroxybenzoic acid was 201.5 °C.

Ethanol was distilled over calcium oxide, and the purity determined from the density was 99.0%.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[15] E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
$t/°\mathrm{C}=20.0$	P. Scharlin

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Solubility of 3-hydroxybenzoic acid in ethanol at 20.0 °C

Solubility[a]	
γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
225.4	1.632

[a] In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

3-Hydroxybenzoic acid was obtained from Shuchardt, reinst.

Ethanol: source and purity not given; relative density d=0.789 (20 °C/4 °C).

Estimated Errors:

Nothing specified. According to the author, the values given are the mean of three independent determinations.

2.1.2.3. 4-Hydroxybenzoic acid

Components:	Evaluators:
(1) Benzoic acid, 4-hydroxy- (p-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 12. Summary of experimental solubility data of 4-hydroxybenzoic acid in ethanol

T/K	c_1/mol dm^{-3}	100w_1	100x_1	Analytical method	Reference
293.2	1.699			Gravimetry	15
298.2			12.13	Spectroscopy	19
340.2		38.75	17.4[a]	Synthetic method	14
409.7		60.9	34.2[a]	Synthetic method	14
457.2		82.9	61.8[a]	Synthetic method	14
486.2		100.0	100.0[a]	Synthetic method	14

[a] The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in n-heptane.

The number of publications: 3

The range of temperature: T/K=293.2−486.2

The units: mass percent, mole fraction, and mol dm^{-3}

Analytical methods: synthetic method, spectrophotometry, and gravimetry

Data for the solubility of 4-hydroxybenzoic acid in ethanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 12). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 5, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

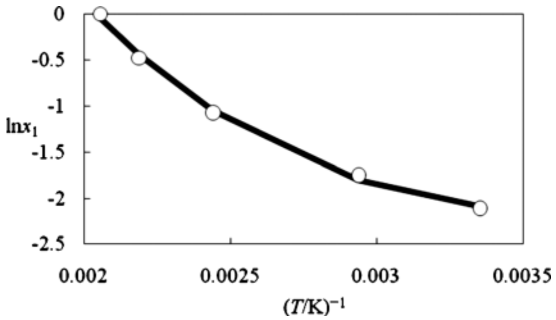

FIG. 5. Fitting curve of Eq. (1) and the observed data for 4-hydroxybenzoic acid in ethanol.

Multiple correlation coefficient: 0.999

Sample size: 5 data points

p-value (F test): 0.003

Constants: $A=4107\pm938$, $B=15.07\pm2.49$, $C=-101.7\pm17.3$

White circles in Fig. 5 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=4107/T+15.07\ln T-101.7$). The observed data fit closely with the calculated values in the range of 298.2−486.2 K, with the multiple correlation coefficient of 0.999, as shown in Fig. 5. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 13 shows the observed data in the range of 298.2−486.2 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 13. Observed data and recommended values calculated according to Eq. (1) for 4-hydroxybenzoic acid in ethanol

T/K	100x_1(obs)	100x_1(rec)
298.2	12.13	12.4
340.2	17.4	16.5
409.7	34.2	35.0
457.2	61.8	64.6
486.2	100	95.6

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy- (p-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[14] S.V. Sidgwick and E.K. Embank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
t/°C=67.0–213.0	A. Goto and H. Miyamoto

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Solubility of 4-hydroxybenzoic acid in ethanol

Temperature	Solubility	
$t/°C$	$100w_1$	$100x_1$ (compiler)
67.0	38.75	17.4
136.5	60.9	34.2
184.0	82.9	61.8
213.0	100.0	100.0

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and purification methods were described in [A. Beerbower, A. Martin, and P.L. Wu, J. Pharm. Sci. **73**, 179 (1984)].

Melting point of 4-hydroxybenzoic acid was 213.0 °C.

Ethanol was distilled over calcium oxide, and the purity determined from the density was 99.0%.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

Original Measurements:

[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:

$t/°C=20.0$

Prepared by:

P. Scharlin

Solubility of 4-hydroxybenzoic acid in ethanol at 20.0 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
243.6	1.699

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

4-Hydroxybenzoic acid was obtained from Shuchardt, purity of 99.5%.

Ethanol source and purity not given; relative density $d=0.789$ (20 °C/4 °C).

Estimated Errors:

Nothing specified. According to the author, the values given are the mean of three independent determinations.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

$t/°C=25$

Prepared by:

A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in ethanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
58.7	0.1213

Auxiliary Information

Methods/Apparatus/Procedure:

A suitable amount of solvent was introduced into screw-capped vials containing an excess amount of the solute. After being sealed with several turns of plastic tape, the vials were submerged in water at 25 °C and shaken. After equilibrium had been attained, each vial was removed, wiped dry, and analyzed. The solutions were transferred to a syringe and filtered using a filter of pore size <1 μm. After suitable dilution, the solutions were assayed using a spectrophotometer. The solubility was determined at least six times for each solvent.

Source and Purity of Materials:

4-Hydroxybenzoic acid was obtained from Matheson, Coleman, and Bell and the acid was recrystallized from aqueous alcohol and dried at 105 °C. Melting point measured by a hot-stage method was 486.85 K.

The solvent was spectrophotometric grade, ACS grade, or redistilled before use.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan

Rensuke Goto, University of Shizuoka, Shizuoka, Japan

Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 14. Summary of experimental solubility data of 4-hydroxybenzoic acid in 1-butanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2		11.54	Spectroscopy	19
305.7	19.50	11.50[a]	Synthetic method	14
335.2	25.08	15.23[a]	Synthetic method	14
389.3	39.45	25.9[a]	Synthetic method	14
440.2	62.4	47.1[a]	Synthetic method	14
467.2	85.5	76.0[a]	Synthetic method	14

[a]The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

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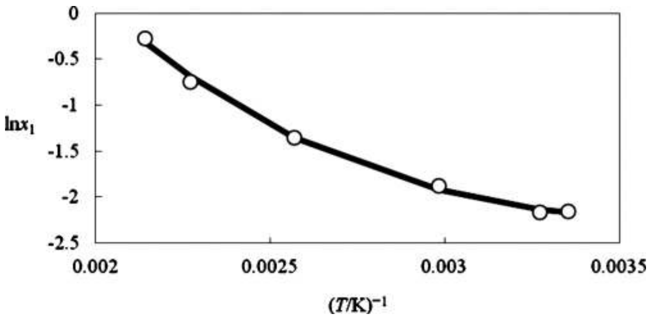

FIG. 6. Fitting curve of Eq. (1) and the observed data for 4-hydroxybenzoic acid in 1-butanol.

The range of temperature: $T/\mathrm{K}=298.2-467.2$

The units: mass percent and mole fraction

Analytical methods: synthetic method and spectrophotometry

Data for the solubility of 4-hydroxybenzoic acid in 1-butanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 14). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 6, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

Multiple correlation coefficient: 0.999

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=4384\pm 858$, $B=15.96\pm 2.33$, $C=-107.8\pm 16.1$

White circles in Fig. 6 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=4384/T+15.96\ln T-107.8$). The observed data fit closely with the calculated values in the range of 298.2–467.2 K, with the multiple correlation coefficient of 0.999, as shown in Fig. 6. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 15 shows the observed data in the range of 298.2–467.2 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 15. Observed data and recommended values calculated according to Eq. (1) for 4-hydroxybenzoic acid in 1-butanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	11.54	11.4
305.7	11.5	11.9
335.2	15.23	14.6
389.3	25.91	25.9
440.2	47.1	50.1
467.2	76.0	72.9

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[14]S.V. Sidgwick and E.K. Embank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°\mathrm{C}=32.5-193.8$	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in 1-butanol

Temperature	Solubility	
$t/°\mathrm{C}$	$100w_1$	$100x_1$ (compiler)
32.5	19.50	11.50
62.0	25.08	15.23
116.1	39.45	25.91
167.0	62.4	47.1
193.8	85.5	76.0

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and purification methods were described in [J. Walker and J.K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of 4-hydroxybenzoic acid was 213.0 °C.

1-Butanol was repeatedly fractionated, and distilled within 0.1 °C.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in 1-butanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	x_1
92.0	0.1154

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

2.1.3. Critical evaluation of the solubility of hydroxybenzoic acids in aromatic compounds

2.1.3.1. Salicylic acid

Components:	**Evaluators:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 16. Summary of experimental solubility data of salicylic acid in benzene

T/K	c_1/mol dm^{-3}	m_1/mol kg^{-1}	$100w_1$	$100x_1$	Analytical method	Reference
284.9		0.0333	0.458	0.2606[a]	Titration ($Ba(OH)_2$)	20
291.4		0.0419	0.576	0.3281[a]	Titration ($Ba(OH)_2$)	20
298.2	0.057 68				Titration	21
301.2				0.5541	Titration ($Ba(OH)_2$)	16
303.7		0.0717	0.981	0.562[a]	Titration ($Ba(OH)_2$)	20
303.8	0.05				Titration (NaOH)	17
307.8		0.0913	1.245	0.717[a]	Titration ($Ba(OH)_2$)	20
309.8		0.1035	1.410	0.814[a]	Titration ($Ba(OH)_2$)	20
317.5			1.92	1.09[a]	Synthetic method	14
322.6		0.1723	2.325	1.360[a]	Titration ($Ba(OH)_2$)	20
337.4		0.319	4.215	2.540[a]	Titration ($Ba(OH)_2$)	20
338.2			5.27	3.05[a]	Synthetic method	14
371.7			20.8	12.9[a]	Synthetic method	14
375.7			5.00	2.89[a]	Fusion method	22
386.2			8.50	4.99[a]	Fusion method	22
387.7			41.1	28.3[a]	Synthetic method	14
400.2			18.95	11.68[a]	Fusion method	22
404.7			64.5	50.4[a]	Synthetic method	14
408.2			31.14	20.37[a]	Fusion method	22
412.7			46.89	33.30[a]	Fusion method	22
413.2			81.3	71.1[a]	Synthetic method	14
418.2			70.0	56.89[a]	Fusion method	22
421.7			84.97	76.17[a]	Fusion method	22
428.2			100.0	100.0[a]	Fusion method	22
432.2			100.0	100.0[a]	Fusion method	14

[a] The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 6

The range of temperature: $T/\mathrm{K}=284.9-432.2$

The units: mass percent, mole fraction, molarity, and mol dm^{-3}

Analytical methods: fusion method, synthetic method, and titration

Data for the solubility of salicylic acid in benzene expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 16). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 7, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

Multiple correlation coefficient: 0.972

Sample size: 23 data points

p-value (F test): 0.000

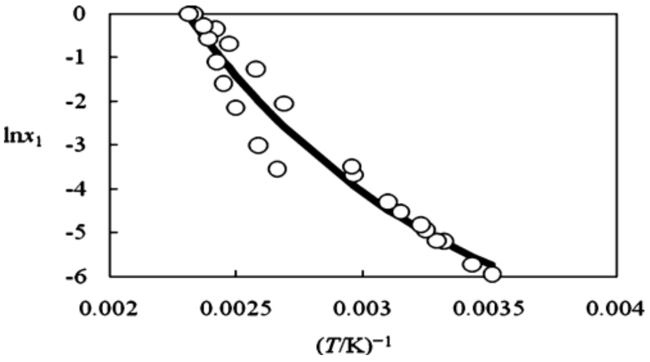

FIG. 7. Fitting curve of Eq. (1) and the observed data for salicylic acid in benzene.

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Constants: $A=8097\pm5739$, $B=36.83\pm16.31$, $C=-242.3\pm112.1$

White circles in Fig. 7 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=8097/T+36.83\ln T-242.3$). The observed data fit closely with the calculated values in the range of 284.9–432.2 K, with the multiple correlation coefficient of 0.972, as shown in Fig. 7. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 17 shows the observed data in the range of 284.9–432.2 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 17. Observed data and recommended values calculated according to Eq. (1) for salicylic acid in benzene

T/K	$100x_1$(obs)	$100x_1$(rec)
284.9	0.2606	0.323
291.4	0.3281	0.394
301.2	0.5541	0.539
303.7	0.562	0.586
307.8	0.717	0.673
309.8	0.814	0.721
317.5	1.09	0.944
322.6	1.36	1.13
337.4	2.54	1.97
338.2	3.05	2.03
371.7	12.9	7.60
375.7	2.89	8.94
386.2	4.99	13.7
387.7	28.3	14.6
400.2	11.68	24.5
404.7	50.4	29.5
408.2	20.37	34.1
412.7	33.3	41.1
413.2	71.1	42.0
418.2	56.89	51.8
421.7	76.17	59.9
428.2	100.0	78.6
432.2	100.0	92.9

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
$t/°C=11.7-64.2$	A. Goto and H. Miyamoto

Solubility of salicylic acid in benzene

Temperature	Solubility[a]	
t/°C	$100w_1$ (compiler)	m_1/mol kg^{-1} (compiler)
11.7	0.460	0.0333
18.2	0.579	0.0419
30.5	0.991	0.0717
34.6	1.261	0.0913
36.6	1.430	0.1035
49.4	2.380	0.1723
64.2	4.40	0.319

[a] In the original paper, the solubility was given as grams per 100 g of solvent.

Auxiliary Information

Methods/Apparatus/Procedure:
Both undersaturation and supersaturation methods were used to obtain the saturated solutions. The solutions were usually agitated by stirrers driven by a small turbine, but at the higher temperature, equilibrium was reached with only occasional agitation by hand. The salicylic acid solutions were titrated directly with barium hydroxide solution using Congo Red as an indicator, after previously diluting with water. The barium hydroxide solution was standardized with pure succinic acid using phenolphthalein as an indicator. In the case of benzene, the solvent was driven off by evaporation under reduced pressure before the titration.

Source and Purity of Materials:
No information was given.

Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Benzene; C_6H_6; [71-43-2]	[14]N.V. Sidgwick and E.K. Ewbank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°C=44.3-159.0$	A. Goto and H. Miyamoto

Solubility of salicylic acid in benzene

Temperature	Solubility	
t/°C	$100w_1$	$100x_1$ (compiler)
44.3	1.92	1.09
65.0	5.27	3.05
98.5	20.8	12.9
114.5	41.1	28.3
131.5	64.5	50.4
140.0	81.3	71.1
159.0	100.0	100.0

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and the purification of salicylic acid were described in [J. Walker and J.K Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of the purified acid was 159.0 °C.

Benzene was freed from thiophene by treatment with sulfuric acid, and frozen out seven times.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).

Variables:

$t/°C=28$

Prepared by:

A. Goto and H. Miyamoto

The solubility of salicylic acid in benzene at 28 °C was reported as $10^2x_1=0.5441$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

Benzene was purified by distillation at its known boiling point.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5%.

Temperature: Nothing specified.

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[21]P. A. Ongley, J. Chem. Soc. **1954**, 3634.

Variables:

$t/°C=25$

Prepared by:

A. Goto and H. Miyamoto

Solubility of salicylic acid in benzene at 25 °C

Solubility	
pS	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
1.239	0.057 68

pS: The negative logarithm of the concentration in the saturated solutions in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:

The solubility was measured by rotating tubes of solvent and solute for at least 8 h at 25 °C (preliminary experiments showed that saturation is reached in 2 h). The solutions were concentrated, if necessary, and titrated with standard alkali, bromothymol-blue-neutralred being used as mixed indicator.

Source and Purity of Materials:

The acid was either of AnalaR standard or was recrystallized before use.

No information on the purity of the organic solvent was reported.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[22]I.L. Krupatkin, Zh. Obsh. Khim. **26**, 3240 (1956) [J. Gen. Chem. USSR (Engl. Transl.) **26**, 3609 (1956)].

Variables:

$t/°C=102.5-155.0$

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in benzene

Crystallization temperature	Benzene		Salicylic acid	
$t/°C$	$100w_2$	$100x_2$ (compiler)	$100w_1$ (compiler)	$100x_1$ (compiler)
102.5	95.00	97.11	5.00	2.89
113.0	91.50	95.01	8.50	4.99
127.0	81.05	88.32	18.95	11.68
135.0	68.14	79.63	31.14	20.37
139.5	53.11	66.70	46.89	33.30
145.0	30.00	43.11	70.00	56.89
148.5	15.03	23.83	84.97	76.17
155.0	0.00	0.00	100.00	100.00

Auxiliary Information

Methods/Apparatus/Procedure:

The system salicylic acid–benzene was investigated by the fusion method.

Source and Purity of Materials:

The melting point of C.P. grade salicylic acid used was 155 °C.

The benzene fraction boiling in the range 90–120 °C was used.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).

Variables:

$t/°C=30.6$

Prepared by:

A. Goto and H. Miyamoto

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Solubility of salicylic acid in benzene at 30.6 °C

Dielectric constant[a]	Solubility[b] γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
2.2	7	0.05

[a] The dielectric constant of the mixture at the maximum solubility of salicylic acid.

[b] In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvent was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Auxiliary Information

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

2.1.3.2. 3-Hydroxybenzoic acid

Components:	Evaluators:
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 18. Summary of experimental solubility data of 3-hydroxybenzoic acid in benzene

T/K	c_1/mol dm^{-3}	m_1/mol kg^{-1}	$100w_1$	$100x_1$	Analytical method	Reference
298.2	0.000 633 9				Titration	21
298.2		0.000 731	1.01	0.005 7	Titration(Ba(OH)$_2$)	20
303.2				0.005 04	Gravimetry	23
307.3		0.001 02		0.007 97	Titration(Ba(OH)$_2$)	20
319.2		0.001 69		0.013 2	Titration(Ba(OH)$_2$)	20
331.2		0.003 15		0.024 6	Titration(Ba(OH)$_2$)	20
337.2		0.004 29		0.033 5	Titration(Ba(OH)$_2$)	20
395.7			1.23	0.699[a]	Synthetic method	14
414.2			2.95	1.69[a]	Synthetic method	14
427.7			5.16	2.99[a]	Synthetic method	14
435.2			10.54	6.24[a]	Synthetic method	14
446.2			22.4	14.0[a]	Synthetic method	14
455.7			41.6	28.7[a]	Synthetic method	14
458.7			62.3	48.3[a]	Synthetic method	14
465.7			83.3	73.8[a]	Synthetic method	14
474.5			100.0	100.0[a]	Synthetic method	14

[a] The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 4

The range of temperature: $T/\text{K}=298.2-474.5$

The units: mass percent, molarity, mole fraction, and mol dm^{-3}

Analytical methods: synthetic method, titration, and gravimetry

Data for the solubility of 3-hydroxybenzoic acid in benzene expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 18). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 8, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

Multiple correlation coefficient: 0.998

Sample size: 15 data points

p-value (F test): 0.000

Constants: $A=18788\pm2831$, $B=-71.40\pm7.60$, $C=-479.6\pm52.7$

White circles in Fig. 8 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=18788/T-71.40\ln T-479.6$). The observed

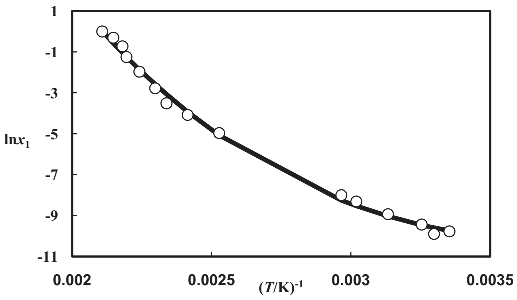

FIG. 8. Fitting curve of Eq. (1) and the observed data for 3-hydroxybenzoic acid in benzene.

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data fit closely with the calculated values in the range of 298.2–474.5 K, with the multiple correlation coefficient of 0.998, as shown in Fig. 8. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 19 shows the observed data in the range of 298.2–474.5 K and the recommended values calculated from Eq. (1) at each temperature.

TABLE 19. Observed data and recommended values calculated according to Eq. (1) for 3-hydroxybenzoic acid in benzene

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	0.0057	0.0059
303.2	0.00504	0.0068
307.3	0.00797	0.0078
319.2	0.0132	0.0120
331.2	0.0246	0.0198
337.2	0.0335	0.0260
395.7	0.699	0.630
414.2	1.69	1.97
427.7	2.99	4.65
435.2	6.24	7.55
446.2	14	15.5
455.7	28.7	28.9
458.7	48.3	35.3
465.7	73.8	56.3
474.5	100	101

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (m-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
$t/°C=25.0–64.0$	A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in benzene

Temperature	Solubility	
$t/°C$	$100w_1$[a] (compiler)	$10^3m_1/\text{mol kg}^{-1}$ (compiler)
25.0	0.0101	0.731
34.1	0.0141	1.02
46.0	0.0234	1.69
58.0	0.0435	3.15
64.0	0.0592	4.29

[a] In the original paper, the solubility was given as grams per 100 g of solvent.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 20 for the binary salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

No information was given.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (m-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	[14]N.V. Sidgwick and E.K. Ewbank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°C=122.5–201.3$	A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in benzene

Temperature	Solubility	
$t/°C$	$100w_1$	$100x_1$ (compiler)
122.5	1.23	0.699
141.0	2.95	1.69
154.5	5.16	2.99
162.0	10.54	6.24
173.0	22.4	14.0
182.5	41.6	28.7
185.5	62.3	48.3
192.5	83.3	73.8
201.3	100.0	100.0

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–n-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The details are given in the compilation of Ref. 14 for the binary salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (m-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Benzene; C_6H_6; [71-43-2]	[21]P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and H. Miyamoto

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Solubility of 3-hydroxybenzoic acid in benzene at 25 °C

Solubility	
pS	10^3c_1/mol dm^{-3} (compiler)
3.198	0.6339

pS: The negative logarithm of the concentration in the saturated solutions in moles per liter.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[23]C.K. Hancock, J.N. Pawloski, and J.P. Idoux, J. Org. Chem. **31**, 3801 (1966).

Variables:

t/°C=30

Prepared by:

A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in benzene at 30 °C

Solubility	
$100x_1$	$100w_1$[a] (compiler)
5.04×10^{-3}	8.99×10^{-3}

[a] In the original paper, the solubility was given as grams of acid per 100 g of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

Equilibrium was approached from the sides of both undersaturation and supersaturation. Solvent and excess solute were mixed at about 25 °C in a ground-glass stoppered conical flask and left in a 30.00 °C water bath, with periodic manual agitation, for several days. In a second flask, solvent and excess solute were mixed and shaken thoroughly at 50 °C and then left in the 30.00 °C water bath. A Soxhlet thimble equipped with a one-hole cork stopper and an inverted, U-shaped delivery tube extending nearly to the bottom of the thimble, was half immersed in the saturated solution. Gentle suction was applied to transfer a part of the saturated solution, free of excess solute, to a second glass-stoppered flask suspended in the 30.00 °C bath. This second flask plus contents were weighed. 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.

Source and Purity of Materials:

Reagent-grade benzene was refluxed over P_2O_5 for 24 h and then distilled. The 3-hydroxybenzoic acid was procured from commercial sources. After two or more recrystallizations from aqueous ethanol, the acid was dried under vacuum over P_2O_5. The melting point was checked.

Estimated Errors:

Solubility (mole fraction units): The average deviation of the replicate values from the mean exceeded 3%.

Temperature: Precision of ±0.02 °C.

2.1.3.3. 4-Hydroxybenzoic acid

Components:

(1) Benzoic acid, 4-hydroxy-, (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) Benzene; C_6H_6; [71-43-2]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan
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Critical Evaluation

TABLE 20. Summary of experimental solubility data of 4-hydroxybenzoic acid in benzene

T/K	c_1/mol dm^{-3}	m_1/mol kg^{-1}	$100w_1$	$100x_1$	Analytical method	Reference
284.2		0.000 143	0.001 97	0.001 12	Titration ($Ba(OH)_2$)	20
298.2				0.003 3	Spectroscopy	19
298.2	0.003 698				Titration	21
303.2			0.001 04	0.005 88	Gravimetry	23
306.2		0.000 413	0.005 71	0.003 22	Titration ($Ba(OH)_2$)	20
322.2		0.001 12	0.015 5	0.008 75	Titration ($Ba(OH)_2$)	20
337.2		0.002 53	0.035 0	0.019 8	Titration ($Ba(OH)_2$)	20
353.2		0.004 78	0.066 0	0.037 3	Titration ($Ba(OH)_2$)	20
405.4			1.04	0.59[a]	Synthetic method	14
430.1			3.03	1.74[a]	Synthetic method	14

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TABLE 20. Summary of experimental solubility data of 4-hydroxybenzoic acid in benzene—Continued

T/K	c_1/mol dm^{-3}	m_1/mol kg^{-1}	$100w_1$	$100x_1$	Analytical method	Reference
438.5			4.30	2.48[a]	Synthetic method	14
451.2			10.3	6.10[a]	Synthetic method	14
464.7			21.0	13.1[a]	Synthetic method	14
468.9			40.6	27.9[a]	Synthetic method	14
472			61.3	47.3[a]	Synthetic method	14
479.2			83.0	73.4[a]	Synthetic method	14
486.2			100.0	100.0[a]	Synthetic method	14

[a] The mole-fraction solubilities were calculated based on w_1.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 5

The range of temperature: $T/\mathrm{K}=284.2-486.2$

The units: mass percent, mole fraction, molarity, and mol dm^{-3}

Analytical methods: synthetic method, titration, spectroscopy, and gravimetry

Data for the solubility of 4-hydroxybenzoic acid in benzene expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 20). The data points closely agree with Eq. (1) over the whole range of temperatures, as shown in Fig. 9, but they deviated from Eq. (2). Multiple regression analysis according to Eq. (1) yielded the following results:

Multiple correlation coefficient: 0.986

Sample size: 16 data points

p-value (F test): 0.000

Constants: $A=15140\pm3294$, $B=60.89\pm8.85$, $C=-408.1\pm61.4$

White circles in Fig. 9 represent the observed data and the black line corresponds to calculated values according to Eq. (1) ($\ln x_1=15140/T+60.89\ln T-408.1$). The observed data fit closely with the calculated values in the range of 284.2–486.2 K, with the multiple correlation coefficient of 0.986, as shown in Fig. 9. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 21 shows the observed data in the range of 284.2–486.2 K and the recommended values calculated from Eq. (1) at each temperature.

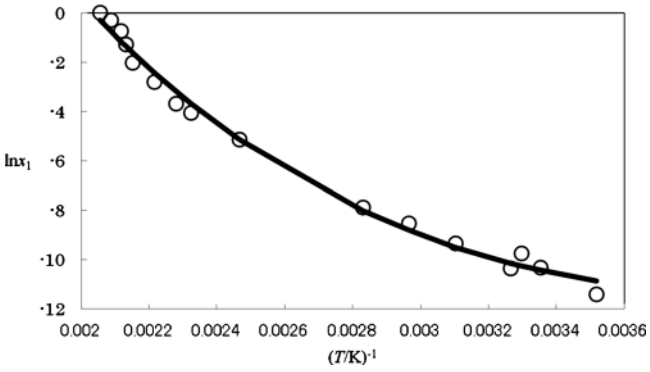

FIG. 9. Fitting curve of Eq. (1) and the observed data for 4-hydroxybenzoic acid in benzene.

TABLE 21. Observed data and recommended values calculated according to Eq. (1) for 4-hydroxybenzoic acid in benzene

T/K	$100x_1$ (obs)	$100x_1$ (rec)
284.2	0.001 12	0.003 53
298.2	0.003 3	0.004 58
303.2	0.005 88	0.005 19
306.2	0.003 22	0.005 63
322.2	0.008 75	0.009 41
337.2	0.019 8	0.016 9
353.2	0.037 3	0.034 5
405.4	0.59	0.547
430.1	1.74	2.36
438.5	2.48	3.93
451.2	6.1	8.58
464.7	13.1	19.9
468.9	27.9	26.0
472	47.3	31.6
479.2	73.4	49.8
486.2	100	77.7

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[20] J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
t/°C=11.0–80.0	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in benzene

Temperature	Solubility		
t/°C	Original data	$100w_1$[a] (compiler)	10^3m_1/mol kg^{-1} (compiler)
11.0	0.001 97	0.001 97	0.143
33.0	0.005 71	0.005 71	0.413
49.0	0.015 5	0.015 5	1.12
64.0	0.035 0	0.035 0	2.53
80.0	0.066 0	0.066 0	4.78

[a] In the original paper, the solubility was given as grams of solute per 100 g of benzene.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 20 for the binary salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

No information was given.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (p-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[14]N.V. Sidgwick and E.K. Ewbank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°C = 132.2-213.0$	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in benzene

Temperature	Solubility	
$t/°C$	$100w_1$	$100x_1$ (compiler)
132.2	1.04	0.59
156.9	3.03	1.74
165.3	4.30	2.48
178.0	10.3	6.10
191.5	21.0	13.1
195.7	40.6	27.9
198.8	61.3	47.3
206.0	83.0	73.4
213.0	100.0	100.0

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–n-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and the purification of 4-hydroxybenzoic acid were described in [J. Walker and J.K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of the purified acid was 213.0 °C.

Benzene was freed from thiophene by treatment with sulfuric acid, and frozen out seven times.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (p-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[21]P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
$t/°C = 25$	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in benzene at 25 °C

Solubility	
pS	$10^3c_1/\text{mol dm}^{-3}$ (compiler)
3.432	0.3698

pS: The negative logarithm of the concentration in the saturated solutions in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

The detail is given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (p-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[23]C.K. Hancock, J.N. Pawloski, and J.P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
$t/°C = 30$	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in benzene at 30 °C

Solubility	
$100x_1$	$100w_1$[a]
5.88×10^{-3}	1.04×10^{-2}

[a] In the original paper, the solubility was given as grams of acid per 100 g of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 23 for the 3-hydroxybenzoic acid–benzene system in Sec. 2.1.3.2.

Source and Purity of Materials:

The details are given in the compilation of Ref. 23 for the 3-hydroxybenzoic acid–benzene system in Sec. 2.1.3.2.

Estimated Errors:

Solubility (mole fraction units): The average deviation of the replicate values from the mean did not exceed 3%.

Temperature: Precision of ±0.02 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (p-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Benzene; C_6H_6; [71-43-2]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C = 25$	A. Goto and R. Goto

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Solubility of 4-hydroxybenzoic acid in benzene at 25 °C

Molar volume of solvent	Solubility
v_2/cm^3 mol^{-1}	$100x_1$
89.4	0.33×10^{-2}

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

2.1.4. Data for hydroxybenzoic acid–organic compound systems

2.1.4.1. Salicylic acid

Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); C_6H_6; [69-72-7] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
$t/°C=28$	A. Goto and H. Miyamoto

The solubility of salicylic acid in *n*-hexane at 28 °C was reported as $10^3x_1=1.11$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

n-Hexane was purified by distillation.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5%.

Temperature: Nothing specified.

Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of salicylic acid in *n*-hexane at 25 °C

Solubility	
10^4x_1	10^3m_1/mol kg^{-1}
4.8	3.4

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 13 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

n-Hexane (ACS) was of reagent grade and used without further purification.

Salicylic acid was recrystallized from hot water.

Estimated Errors:

Nothing specified.

Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) *n*-Decane (decane); $C_{10}H_{22}$; [124-18-5]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of salicylic acid in *n*-decane at 25 °C

Solubility	
10^4x_1	10^3m_1/mol kg^{-1}
6.2	3.2

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 13 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

Decane of reagent grade was purified by passing the solvent through a column of silica gel followed by distillation from sodium under reduced pressure.

Salicylic acid was recrystallized from hot water.

Estimated Errors:

Nothing specified.

Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) *n*-Dodecane (dodecane); $C_{12}H_{26}$; [112-40-3]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

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Solubility of salicylic acid in *n*-dodecane at 25 °C

Solubility	
10^4x_1	10^3m_1/mol kg^{-1}
6.4	2.8

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 13 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

Dodecane of reagent grade was passed through a column of silica gel.

Salicylic acid was recrystallized from hot water.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) *n*-Hexadecane (hexadecane); $C_{16}H_{34}$; [544-76-3]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared By:**
$t/°C=25$	A. Goto and R. Goto

Solubility of salicylic acid in *n*-hexadecane at 25 °C

Solubility	
10^4x_1	10^3m_1/mol kg^{-1}
10.4	3.0

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 13 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

n-Hexadecane of reagent grade was purified by passing the solvent through a column of silica gel followed by distillation from sodium under reduced pressure.

Salicylic acid was recrystallized from hot water.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared By:**
$t/°C=25$	A. Goto and R. Goto

Solubility of salicylic acid in isooctane at 25 °C

Solubility	
10^4x_1	10^3m_1/mol kg^{-1}
3.8	2.3

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 13 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

Isooctane of reagent grade was distilled over sodium. Salicylic acid was recrystallized from hot water.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[21]P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared By:**
$t/°C=25$	A. Goto and H. Miyamoto

Solubility of salicylic acid in cyclohexane at 25 °C

Solubility	
pS	10^3c_1/mol dm^{-3} (compiler)
2.192	6.427

pS: The negative logarithm of the concentration in the saturated solutions in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

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Solubility of salicylic acid in cyclohexane at 25 °C

Solubility	
10^4x_1	$10^3m_1/\mathrm{mol\ kg^{-1}}$
4.3	4.0

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 13 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:
Cyclohexane of reagent grade was distilled over phosphorus pentaoxide.
Salicylic acid was recrystallized from hot water.

Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	[24]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	E. Königsberger and L.-C. Königsberger

The solubility of salicylic acid in chloroform at 25 °C was reported as $c_1/\mathrm{mol\ dm^{-3}}=0.157$.

Auxiliary Information

Methods/Apparatus/Procedure:
Excess solid and solvents were shaken in a thermostat at 25 °C until saturation (time not specified). After the solid phase settled, a certain volume of the clear liquid was pipetted, in which the acid concentration was determined by titration (details not given).

Source and Purity of Materials:
Not stated.

Estimated Errors:
Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
$t/°\mathrm{C}=28$	A. Goto and H. Miyamoto

The solubility of salicylic acid in chloroform at 28 °C was reported as $10^2x_1=2.679$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid was twice recrystallized.
Organic solvents were purified by distillation.

Estimated Errors:
Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5%.
Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	[21]P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and H. Miyamoto

Solubility of salicylic acid in chloroform at 25 °C

Solubility	
pS	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
0.680	0.2089

pS: The negative logarithm of the concentration in the saturated solutions in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:
The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
$t/°\mathrm{C}=30$	A. Goto and R. Goto

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Solubility of salicylic acid in chloroform at 30 °C

Solubility	
x_1[a]	m_1/mol kg^{-1}
1.3×10^{-3}	1.6×10^{-1}

[a] The value was estimated by the author from A. Seidell, *Solubilities of Organic Compounds*, Vol. II, 3rd Ed. (Van Nostrand, New York, 1941).

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 13 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

Salicylic acid was recrystallized in hot water.

Chloroform was washed with distilled water five to six times, dried over powdered calcium chloride overnight, filtered, and distilled over phosphorous pentoxide.

Estimated Errors:

Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Methane, tetrachloro- (tetrachloromethane, carbon tetrachloride); CCl_4; [56-23-5]	[24] W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
t/°C=25	E. Königsberger and L.-C. Königsberger

The solubility of salicylic acid in carbon tetrachloride at 25 °C was reported as c_1/mol dm^{-3}=0.030.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 24 for the binary salicylic acid–chloroform system earlier in this section.

Source and Purity of Materials:

Not stated.

Estimated Errors:

Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Methane, tetrachloro- (tetrachloromethane, carbon tetrachloride); CCl_4; [56-23-5]	[16] P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
t/°C=28	A. Goto and H. Miyamoto

The solubility of salicylic acid in carbon tetrachloride at 28 °C was reported as $100x_1$=0.3803.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

Organic solvent was purified by distillation.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5%.

Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Methane, tetrachloro- (tetrachloromethane, carbon tetrachloride); CCl_4; [56-23-5]	[21] P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
t/°C=25	A. Goto and H. Miyamoto

Solubility of salicylic acid in carbon tetrachloride at 25 °C

Solubility	
pS	c_1/mol dm^{-3} (compiler)
1.644	0.02270

pS: The negative logarithm of the concentration in the saturated solutions in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:

Nothing specified.

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Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethane, 1,1,2,2-tetrachloro- (1,1,2,2-tetrachloroethane, tetrachloroethane); $C_2H_2Cl_4$; [79-34-5]	[24]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
$t/°C=25$	E. Königsberger and L.-C. Königsberger

The solubility of salicylic acid in tetrachloroethane at 25 °C was reported as $c_1/\text{mol dm}^{-3}=0.151$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 24 for the salicylic acid–chloroform system earlier in this section.

Source and Purity of Materials:

Not stated.

Estimated Errors:

Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethane, pentachloro- (1,1,1,2,2-pentachloroethane, pentachloroethane); C_2HCl_5; [76-01-7]	[24]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
$t/°C=25$	E. Königsberger and L.-C. Königsberger

The solubility of salicylic acid in pentachloroethane at 25 °C was reported as $c_1/\text{mol dm}^{-3}=0.077$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 24 for the salicylic acid–chloroform system earlier in this section.

Source and Purity of Materials:

Not stated.

Estimated Errors:

Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethene, trichloro- (1,1,2-trichloroethene, trichloroethylene); C_2HCl_3; [79-01-6]	[24]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
$t/°C=25$	E. Königsberger and L.-C. Königsberger

The solubility of salicylic acid in trichloroethylene at 25 °C was reported as $c_1/\text{mol dm}^{-3}=0.110$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 24 for the salicylic acid–chloroform system earlier in this section.

Source and Purity of Materials:

Not stated.

Estimated Errors:

Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethene, trichloro- (1,1,2-trichloroethene, trichloroethylene); C_2HCl_3; [79-01-6]	[25]D.H. Wester and A. Bruins, Pharm. Weekblad. **51**, 1443 (1914).
Variables:	**Prepared by:**
$t/°C=15$	E. Königsberger and L.-C. Königsberger

Solubility of salicylic acid in trichloroethylene at 15 °C

Solubility	
$100w_1$	$m_1/\text{mol kg}^{-1}$ (compiler)
0.757	0.0548

Auxiliary Information

Methods/Apparatus/Procedure:

A large excess of the solid substance was continuously shaken with the solvent in a water bath of 30 °C for 1 h. Then, the solution was brought to a cellar with a constant temperature of 15 °C and, after keeping it there under repeated shaking for at least 48 h, the quantity of the dissolved substance was determined (details not specified). The undissolved substance was used for a second solubility experiment, and then the remaining substance for a third one. The result of the first experiment was discarded so that the value reported is the average of the other two determinations.

Source and Purity of Materials:

Not stated.

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Estimated Errors:

Solubility: Nothing specified.

Temperature: Uncertainty of ±2 K.

Components:	**Original Measurements:**
(1) Benzoic acid 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethene, tetrachloro- (1,1,2,2-tetrachloroethene, tetrachloroethylene); C_2Cl_4; [127-18-4]	[24]W. Herz and W. Rathmann, Z. Elektrochem. **19**, 887 (1913).
Variables:	**Prepared by:**
$t/°C=25$	E. Königsberger and L.-C. Königsberger

The solubility of salicylic acid in tetrachloroethylene at 25 °C was reported as $c_1/\text{mol dm}^{-3}=0.080$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 24 for the salicylic acid–chloroform system earlier in this section.

Source and Purity of Materials:

Not stated.

Estimated Errors:

Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[26]E. Savorro, Atti accad. sci. Torino **48**, 948 (1914) [Chem. Abs. **8**, 340 (1914)].
Variables:	**Prepared by:**
$t/°C=15$	A. Goto and H. Miyamoto

Solubility of salicylic acid in methanol at 15 °C

Solubility[a]			
Original data	$100w_1$ (compiler)	$m_1/\text{mol kg}^{-1}$ (compiler)	x_1 (compiler)
398.66	28.503	2.8863	0.0846

[a] In the original paper, the solubility was given as grams per 1000 g of methanol.

Auxiliary Information

Methods/Apparatus/Procedure:

The solubility of salicylic acid in water was determined in Pawlewski″s apparatus [B. Pawlewski, Ber. Dtsch. Chem. Ges. **32**, 1040 (1899)]. The salicylic acid content was determined with standardized sodium hydroxide solution. The water and salicylic acid were placed in the test tube. The tube was equipped with a condenser and a siphon glass tube, and connected with a weighing bottle equipped with a condenser. The apparatus was placed into a large thermostated glass beaker to mix the water and salicylic acid, and air was bubbled through the mixture. After equilibrium was established, the saturated solution in the tube was filtered into the weighing tube through the siphon tube equipped with a cotton wool filter. The apparatus was removed from the large beaker, cooled and/or dried, and the bottle was weighed. Salicylic acid was determined gravimetrically after evaporation of the solvent.

Source and Purity of Materials:

Salicylic acid was recrystallized before use.

Estimated Errors:

Solubility: Precision of ±1.5%.

Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
$t/°C=28$	A. Goto and H. Miyamoto

The solubility of salicylic acid in methanol at 28 °C was reported as $x_1=0.1252$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

Methanol was purified by distillation.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5%.

Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
$t/°C=20.0$	P. Scharlin

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Solubility of salicylic acid in methanol at 20.0 °C

Solubility[a]	
γ_1 / g dm^{-3} (compiler)	c_1 / mol dm^{-3} (compiler)
331.3	2.398

[a] In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was obtained from Shuchardt, DAB6.

Methanol: source and purity not given; relative density $d = 0.792$ (20 °C/4 °C).

Estimated Errors:

Nothing specified. The value given was the mean of three independent determinations.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:
[17] A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).

Variables:
t / °C = 30.6

Prepared by:
A. Goto and R. Goto

Solubility of salicylic acid in methanol at 30.6 °C

	Solubility[a]	
Dielectric constant of solvent	γ_1 / g dm^{-3} (compiler)	c_1 / mol dm^{-3} (compiler)
32.6	299	2.16

[a] In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

The dielectric constant of the solvent was measured by a resonance method at 25 °C.

Source and Purity of Materials:

Methanol was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

Original Measurements:
[16] P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).

Variables:
t / °C = 28

Prepared by:
A. Goto and H. Miyamoto

The solubility of salicylic acid in 1-propanol at 28 °C was reported as $x_1 = 0.1438$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

1-Propanol was purified by distillation.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5%.

Temperature: Nothing specified.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

Original Measurements:
[15] E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:
t / °C = 20.0

Prepared by:
P. Scharlin

Solubility of salicylic acid in 1-propanol at 20.0 °C

Solubility[a]	
γ_1 / g dm^{-3} (compiler)	c_1 / mol dm^{-3} (compiler)
222.5	1.611

[a] In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was obtained from Shuchardt, DAB6.

1-Propanol: source and purity not given; relative density $d = 0.804$ (20 °C/4 °C).

Estimated Errors:

Nothing specified. The value given is the mean of three independent determinations.

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Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
$t/°C=30.6$	A. Goto and R. Goto

Solubility of salicylic acid in 1-propanol at 30.6 °C

	Solubility[a]	
Dielectric constant of solvent	γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
20.1	287	2.08

[a]In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvent was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[18]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:**
$T/K=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 1-propanol at 298.15 K was reported as $x_1=0.1636$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was described in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

1-Propanol (Aldrich, 99+%, anhydrous) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]	[18]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:**
$T/K=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 1-pentanol at 298.15 K was reported as $x_1=0.1611$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was described in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

1-Pentanol (Aldrich, 99+%) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	Original Measurements:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[18]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:**
$T/K=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 1-octanol at 298.15 K was reported as $x_1=0.2143$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was described in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

1-Octanol (Aldrich, 99+%, anhydrous) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

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Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Propanol (propan-2-ol, isopropyl alcohol); C_3H_8O; [67-63-0]	[18]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:**
$T/\mathrm{K}=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 2-propanol at 298.15 K was reported as $x_1=0.1789$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was described in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

2-Propanol (Aldrich, 99+%, anhydrous) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Butanol (butan-2-ol, *sec*-butyl alcohol); $C_4H_{10}O$; [78-92-2]	[18]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:**
$T/\mathrm{K}=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 2-butanol at 298.15 K was reported as $x_1=0.1869$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was described in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

2-Butanol (Aldrich, 99+ %, anhydrous) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Methyl-1-propanol (2-methylpropan-1-ol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]	[18]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:**
$T/\mathrm{K}=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 2-methyl-1-propanol at 298.15 K was reported as $x_1=0.1430$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was described in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

2-Methyl-1-propanol (Aldrich, 99.5%, anhydrous) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Methyl-2-propanol (2-methylpropan-2-ol, *tert*-butyl alcohol); $C_4H_{10}O$; [75-65-0]	[18]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:**
$T/\mathrm{K}=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 2-methyl-2-propanol at 298.15 K was reported as $x_1=0.2193$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was described in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

2-Methyl-2-propanol (Arco Chemical Company, 99+%) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

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Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
$t/°C=30.6$	A. Goto and R. Goto

Solubility of salicylic acid in cyclohexanol at 30.6 °C

Dielectric constant of solvent	Solubility[a] $\gamma_1/\mathrm{g\,dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\,dm^{-3}}$ (compiler)
15.0	217	1.57

[a]In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvent was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Benzyl alcohol (phenylmethanol); C_7H_8O; [100-51-6]	[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
$t/°C=30.6$	A. Goto and R. Goto

Solubility of salicylic acid in benzyl alcohol at 30.6 °C

Dielectric constant of solvent	Solubility[a] $\gamma_1/\mathrm{g\,dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\,dm^{-3}}$ (compiler)
13.0	203	1.47

[a]In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Benzyl alcohol was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Organic solvents: 1,2-Propanediol (propane-1,2-diol, propylene glycol); $C_3H_8O_2$; [57-55-6] 1,2-Ethanediol (ethan-1,2-diol, ethylene glycol); $C_2H_6O_2$; [107-21-1] 1,2,3-Propanetriol (propane-1,2,3-triol, glycerol); $C_3H_8O_3$; [56-81-5]	[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
$t/°C=30.6$	A. Goto and R. Goto

Solubility of salicylic acid in diols and triol at 30.6 °C

Solvent	Dielectric constant of solvent	Solubility[a] $\gamma_1/\mathrm{g\,dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\,dm^{-3}}$ (compiler)
Propylene glycol	33.0	118	0.854
Ethylene glycol	37.7	42	0.30
Glycerol	42.5	15	0.11

[a]In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvents were purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

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Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethane, 1,1′-oxybis- (ethoxyethane, diethyl ether); $C_4H_{10}O$; [60-29-7]	[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
$t/°C=17$	A. Goto and H. Miyamoto

Solubility of salicylic acid in diethyl ether at 17 °C

Solubility[a]		
Original data	$\gamma_1/g\ dm^{-3}$ (compiler)	$c_1/mol\ dm^{-3}$ (compiler)
23.4	234	1.69

[a]In the original paper, the solubility was given as grams of salicylic acid per 100 cm^3 of diethyl ether solution at 17 °C. The mass concentration, $\gamma_1 = m_1/V$, was calculated by the compiler, where m_1 is the mass of component 1 and V is the total volume of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–benzene system in Sec. 2.1.2.1.

Source and Purity of Materials:

No information was given.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Ethane, 1,1′-oxybis- (ethoxyethane, diethyl ether); $C_4H_{10}O$; [60-29-7]	[13]H.-L. Fung and T. Higuchi, J. Pharm. Sci. **60**, 1782 (1971).
Variables:	**Prepared by:**
$t/°C=20$	A. Goto and H. Miyamoto

Solubility of salicylic acid in diethyl ether at 20 °C

Solubility	
x_1	$m_1/mol\ kg^{-1}$
2.5×10^{-1}[a]	2.4[b]

[a]The value was estimated by the author from A. Seidell, *Solubilities of Organic Compounds*, 3rd Ed. (Van Nostrand, New York, 1941), Vol. II.

[b]The value was estimated by the author from *The Merck Index*, 8th ed. (Merck, Rahway, NJ, 1968).

Auxiliary Information

Methods/Apparatus/Procedure:

Not stated.

Source and Purity of Materials:

Not stated.

Estimated Errors:

Not stated.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Butane, 1,1′-oxybis- (2-butoxy ethanol, *n*-butyl ether); $C_8H_{18}O$; [142-96-1]	[18]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:**
$T/K=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in *n*-dibutyl ether at 298.15 K was reported as $x_1=0.091\,85$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

n-Dibutyl ether (Aldrich, 99 %) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]	[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).
Variables:	**Prepared by:**
$t/°C=23$	A. Goto and H. Miyamoto

Solubility of salicylic acid in acetone at 23 °C

Solubility[a]		
Original data	$\gamma_1/g\ dm^{-3}$ (compiler)	$c_1/mol\ dm^{-3}$ (compiler)
31.3	313	2.27

[a]In the original paper, the solubility was given as grams of salicylic acid per 100 cm^3 of acetone solution at 23 °C. The mass concentration, $\gamma_1=m_1/V$, was calculated by the compiler, where m_1 is the mass of component 1 and V is the total volume of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 20 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:
No information was given.

Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]	[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
$t/°C=28$	A. Goto and H. Miyamoto

The solubility of salicylic acid in acetone at 28 °C was reported as $x_1=0.1906$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid was twice recrystallized.
Acetone was purified by distillation at its known boiling point.

Estimated Errors:
Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5 %.
Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]	[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
$t/°C=20$	P. Scharlin

Solubility of salicylic acid in acetone at 20 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
294.4	2.131

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid was obtained from Shuchardt, DAB6.
Acetone: source and purity not given; relative density $d=0.791$ (20 °C/4 °C)

Estimated Errors:
Nothing specified. The value given is the mean of three independent determinations.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]	[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).
Variables:	**Prepared by:**
$t/°C=30.6$	A. Goto and R. Goto

Solubility of salicylic acid in acetone at 30.6 °C

	Solubility[a]	
Dielectric constant of solvent	$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
24.3	377	2.73

[a]In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
The solvent was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]	[18]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:**
$T/K=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in acetone at 298.15 K was reported as $x_1=0.1817$.

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Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid is given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Acetone (Aldrich, HPLC, 99.9+%) was stored over molecular sieves before use.

Estimated Errors:
Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) 2-Butanone (butan-2-one, methyl ethyl ketone); C_4H_8O; [78-93-3]

Original Measurements:
[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:
$t/°C=20$

Prepared by:
P. Scharlin

Solubility of salicylic acid in 2-butanone at 20 °C

Solubility[a]	
γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
235.6	1.706

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid was obtained from Shuchardt, DAB6.

2-Butanone: source and purity not given; relative density $d=0.805$ (20 °C/4 °C).

Estimated Errors:
Nothing specified. The value given is the mean of three independent determinations.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) 2-Butanone (butan-2-one, methyl ethyl ketone); C_4H_8O; [78-93-3]

Original Measurements:
[18]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:
A. Goto and H. Miyamoto

The solubility of salicylic acid in 2-butanone at 298.15 K was reported as $x_1=0.1852$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid is given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

2-Butanone (Aldrich, HPLC, 99.5 %) was stored over molecular sieves before use.

Estimated Errors:
Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) 2-Pentanone (pentan-2-one, methyl propyl ketone); $C_5H_{10}O$; [107-87-9]

Original Measurements:
[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:
$t/°C=20$

Prepared by:
P. Scharlin

Solubility of salicylic acid in 2-pentanone at 20 °C

Solubility[a]	
γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
209.2	1.515

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid was obtained from Shuchardt, DAB6.

2-Pentanone: source and purity not given; relative density $d=0.812$ (15 °C/15 °C).

Estimated Errors:
Nothing specified. The value given is the mean of three independent determinations.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]

Original Measurements:
[18]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:
A. Goto and H. Miyamoto

The solubility of salicylic acid in cyclohexanone at 298.15 K was reported as $x_1=0.2301$.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid is given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Cyclohexanone (Aldrich, 99.8%) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Acetates: Acetic acid, ethyl ester (ethyl acetate); $C_4H_8O_2$; [141-78-6] Acetic acid, butyl ester (butyl acetate); $C_6H_{12}O_2$; [123-86-4]	[18]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:**
$T/\mathrm{K}=298.15$	A. Goto and H. Miyamoto

Solubility of salicylic acid in acetates at 298.15 K

	Solubility
Solvent	x_1
Ethyl acetate	0.1425
Butyl acetate	0.1363

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid is given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Ethyl acetate (Aldrich, HPLC, 99.9 %) and butyl acetate (Aldrich, HPLC, 99.7 %) were stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Benzene derivatives: Benzene, methyl- (toluene); C_7H_8; [108-88-3] Benzene, 1,3-dimethyl- (1,3-xylene, *m*-xylene); C_8H_{10}; [108-38-3] Benzene, chloro- (chlorobenzene); C_6H_5Cl; [108-90-7] Benzene, nitro- (nitrobenzene); $C_6H_5NO_2$; [98-95-3]	[16]P.G. Desai and A.M. Patel, J. Indian Chem. Soc. **12**, 131 (1935).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=28$	A. Goto and H. Miyamoto

Solubility of salicylic acid in benzene derivatives at 28 °C

	Solubility
Solvent	10^2x_1
Toluene	0.6052
m-Xylene	0.6554
Chlorobenzene	0.7903
Nitrobenzene	2.509

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the binary salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid was twice recrystallized.

The organic solvents were purified by distillation.

Estimated Errors:

Solubility: Three readings were taken in each case and the mean was taken. It was found by blank experiments (on solute-free solvent) that this method gave reliable results; the precision being less than 0.5 %.

Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Phenol; C_6H_6O; [108-95-2]	[27]C.R. Bailey, J. Chem. Soc. Trans. **126**, 1951 (1925).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=38.16-160.4$	A. Goto and H. Miyamoto

Solubility of salicylic acid in phenol

Temperature	Solubility		Eutectic temperature[a]	Duration of eutectic halt[b]
$t/{}^\circ\mathrm{C}$	$100w_1$	$100x_1$ (compiler)	$t/{}^\circ\mathrm{C}$	min
40.80	0.0	0.0	—	—
39.95	1.64	1.12	—	—
39.12	3.17	2.18	38.10	18

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Solubility of salicylic acid in phenol

Temperature	Solubility		Eutectic temperature[a]	Duration of eutectic halt[b]
$t/°\mathrm{C}$	$100w_1$	$100x_1$ (compiler)	$t/°\mathrm{C}$	min
38.47	4.39	3.03	38.16	25
38.16	5.00	3.46	38.16[c]	28.5
45.9	7.38	5.15	38.18	28
55.6	10.09	7.10	38.07	27.5
65.6	14.2	10.1	37.9	26
89.2	27.5	20.5	38.0	23
113.5	46.0	36.7	—	—
128.7	60.0	50.5	38.0	—
147.2	81.8	75.4	—	—
157.0	94.9	92.7	—	—
160.4	100.0	100.0	—	—

[a] The mixture of salicylic acid and phenol corresponds to a eutectic system and the temperature at which the solid phase begins to appear is called the eutectic temperature.

[b] The eutectic halt (or arrest) means the time during which the solid phase appears at the eutectic temperature as the mixture is cooled.

[c] In this paper, the eutectic point was assumed to be 5.0 % salicylic acid and 38.16 °C by the eutectic halt.

Auxiliary Information

Methods/Apparatus/Procedure:

The synthetic method was used. At higher temperatures near the melting point of salicylic acid, mixtures of phenol and salicylic acid were sealed in glass tubes, and the temperatures of appearance and disappearance of solid phase were noted. At lower temperature, the eutectic halt times (or arrests) were measured. Salicylic acid was directly estimated with barium hydroxide; the indicator chosen was *p*-nitrophenol with titration to a color match.

Source and Purity of Materials:

Commercial salicylic acid was recrystallized from water four times. The physiologically pure salicylic acid was dissolved in a hot mixture of phenol and water, and the solution was slowly cooled. After the product was recrystallized twice, the m.p. of the purified product was 158.7 °C. When allowance was made for the exposed stem of the thermometer, the m.p. was reported as 160.4 °C.

The phenol crystals were purchased from British Drug Houses and were distilled twice. The m.p. of the product was 40.8 °C.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Benzoic acid, 2-amino- (2-aminobenzoic acid, anthranilic acid); $C_7H_7NO_2$; [118-92-3]	[28] I.L. Krupatkin, Sbornik Statei Obshchei po Khim., Akad. Nauk S.S.S.R. **2**, 1221 (1953)
Variables:	**Prepared by:**
Composition and temperature	H. Miyamoto and A. Goto

Solubility of salicylic acid in 2-aminobenzoic acid

Crystallization temperature	Aminobenzoic acid		Solubility of salicylic acid	
$t/°\mathrm{C}$	$100w_2$	$100x_2$	$100w_1$	$100x_1$
155.0	0.00	0.00	100.00	100.00
148.0	10.87	10.94	89.13	89.06
141.5	20.91	21.03	79.09	78.97
134.0	29.73	29.88	70.27	70.12
123.0	40.02	40.19	59.98	59.81
113.0	49.34	49.52	50.66	50.48
110.0[a]	53.00	53.18	47.00	46.82
112.0	55.12	55.30	44.88	44.70
117.0	60.06	60.23	39.94	39.77
122.0	65.15	65.31	34.85	34.69
129.0	74.71	74.85	35.29	25.15
136.0	85.13	85.22	14.87	14.78
145.0	100.00	100.00	0.00	0.00

[a] Eutectic point

Auxiliary Information

Methods/Apparatus/Procedure:

The experiment was performed by the fusion method.

Source and Purity of Materials:

Chemically pure grade salicylic acid with m.p. of 155 °C and chemically pure grade aminobenzoic acid with m.p. of 145 °C were used.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	[18] 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:**
$T/\mathrm{K}=298.15$	A. Goto and H. Miyamoto

The solubility of salicylic acid in 1,4-dioxane at 298.15 K was reported as $x_1=0.294$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

Salicylic acid is given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

1,4-Dioxane (Aldrich, 99.8% anhydrous) was stored over molecular sieves before use.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

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Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Furan, tetrahydro- (oxolane, tetrahydrofuran); C_4H_8O; [109-99-9]

Original Measurements:
[18]K.M. De Fina, T.L. Sharp, L.E. Roy, and W.E. Acree Jr., J. Chem. Eng. Data **44**, 1262 (1999).

Variables:
$T/\mathrm{K}=298.15$

Prepared by:
A. Goto and H. Miyamoto

The solubility of salicylic acid in tetrahydrofuran at 298.15 K was reported as $x_1=0.3642$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
Salicylic acid is given in the compilation of Ref. 18 for the salicylic acid–1-butanol system in Sec. 2.1.2.1.

Tetrahydrofuran (Aldrich, 99.9% anhydrous) was stored over molecular sieves before use.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Aminopyrine (4-(dimethylamino)-1,5-dimethyl-2-phenylpyrazol-3-one); $C_{13}H_{17}N_3O$; [58-15-1]

Original Measurements:
[29]I.L. Krupatkin, Zh. Obsh. Khim. **26**, 1050 (1956) [J. Gen. Chem. USSR (Engl. Transl.) **26**, 1197 (1956)].

Variables:
$t/{}^\circ\mathrm{C}=82.0–104.0$

Prepared by:
H. Miyamoto and A. Goto

Solubility of salicylic acid in aminopyrine

Crystallization temperature	Solubility	
$t/{}^\circ\mathrm{C}$	$100w_1$	$100x_1$
82.0	51.5	64.0
83.0	52.0	64.5
84.0	50.0	62.6
87.0	18.0	26.9
88.0	20.0	29.5
90.0	45.0	57.8
90.0	55.0	67.2
91.0	15.0	22.8
91.0	25.0	35.8
92.0	43.0	55.8
93.0	28.0	39.4
93.0	60.0	71.5
93.5	63.0	74.0
94.5	30.0	41.8
95.0	40.0	52.7
96.5	39.0	51.7
97.0	35.0	47.4
97.0	37.4	50.0
98.0	10.0	15.7
99.0	64.0	74.9
103.0	65.0	75.7
104.0	5.0	8.1
107.0	66.0	76.5
108.0	0.0	0.0
116.0	38.0	50.6
124.0	70.0	79.6
134.0	75.0	83.4
142.0	80.0	87.0
152.0	90.0	93.8
155.0	100.0	100.0

Auxiliary Information

Methods/Apparatus/Procedure:
The binary aminopyrine–salicylic acid system was studied by the fusion method.

Source and Purity of Materials:
Parmacopoeia aminopyrine with m.p. of 108 °C and c.p. salicylic acid with m.p. of 155 °C were used.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Ethanol, 2-ethoxy- (2-ethoxyethanol, ethyl cellosolve); $C_4H_{10}O_2$; [110-80-5]

Original Measurements:
[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).

Variables:
$t/{}^\circ\mathrm{C}=30.6$

Prepared by:
A. Goto and R. Goto

Solubility of salicylic acid in ethyl cellosolve at 30.6 °C

Dielectric constant of solvent	Solubility[a]	
	$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
14.5	425	3.08

[a] In the original paper, the solubility was given as mg/ml of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 16 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvent was purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

2.1.4.2. 3-Hydroxybenzoic acid

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) *n*-Heptane; C_7H_{16}; [142-82-5]	[14]N.V. Sidgwick and E.K. Ewbank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/°C=176.0$ and 197.0	A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in *n*-heptane

Temperature	Solubility	
$t/°C$	$100w_1$	$100x_1$ (compiler)
197.0(liq.)	2.00	1.46
176.0	0.86	0.63
197.0	Triple point	

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and the purification of 3-hydroxybenzoic acid were described in [J. Walker and J. K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of the purified acid was 201.5 °C.

n-Heptane was a specimen from *Pinus sabiniana*, which had been purified by the method of Thorpe [T. E. Thorpe, J. Chem. Soc. **35**, 296 (1879)] by treatment with sulfuric and nitric acids, and distillation.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[21]P. A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in cyclohexane at 25 °C.

Solubility	
pS	$c_1/\text{mol dm}^{-3}$ (compiler)
>6.000	$<1.000\times10^{-6}$

pS: The negative logarithm of the concentration in the saturated solutions in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[23]C.K. Hancock, J.N. Pawloski, and J.P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
$t/°C=30$	A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in cyclohexane at 30 °C

Solubility[a]	
x_1 (compiler)	$100w_1$ (compiler)
9.73×10^{-6}	1.69×10^{-3}

[a] In the original paper, the solubility was given as grams of acid per 100 g of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 23 for the 3-hydroxybenzoic acid–benzene system in Sec. 2.1.3.2.

Source and Purity of Materials:

The details are given in the compilation of Ref. 23 for the 3-hydroxybenzoic acid–benzene system in Sec. 2.1.3.2.

Estimated Errors:

Solubility (mole fraction units): The average deviation of the replicate values from the mean exceeds 3% only in the case of 5.5% for 3-hydroxybenzoic acid in cyclohexane.

Temperature: Precision of ±0.02 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[26]E. Savarro, Atti Accad. Sci. Torino **48**, 948 (1914) [Chem. Abs. **8**, 340 (1914)].

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Variables:
$t/°\text{C}=15$

Prepared by:
A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in methanol at 15 °C

Solubility[a]		
Original data	$100w_1$ (compiler)	$m_1/\text{mol kg}^{-1}$ (compiler)
535.80	34.887	3.8792

[a] In the original paper, the solubility was given as grams per 1000 g of methanol.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 26 for the binary salicylic acid–methanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
3-Hydroxybenzoic acid was recrystallized.

Estimated Errors:
Solubility: Precision of ±1.5%.
Temperature: Nothing specified.

Components:
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9]
(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:
[15] E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:
$t/°\text{C}=20.0$

Prepared by:
P. Scharlin

Solubility of 3-hydroxybenzoic acid in methanol at 20.0 °C

Solubility[a]	
$\gamma_1/\text{g dm}^{-3}$ (compiler)	$c_1/\text{mol dm}^{-3}$ (compiler)
278.6	2.017

[a] In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
3-Hydroxybenzoic acid was obtained from Shuchardt, reinst.

The source and purity of methanol was not given; relative density $d=0.792$ (20 °C/4 °C).

Estimated Errors:
Nothing specified. The values given are the mean of three independent determinations.

Components:
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9]
(2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

Original Measurements:
[15] E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:
$t/°\text{C}=20.0$

Prepared by:
P. Scharlin

Solubility of 3-hydroxybenzoic acid in 1-propanol at 20.0 °C

Solubility[a]	
$\gamma_1/\text{g dm}^{-3}$ (compiler)	$c_1/\text{mol dm}^{-3}$ (compiler)
163.4	1.183

[a] In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
3-Hydroxybenzoic acid was obtained from Shuchardt, reinst.

The source and purity of 1-propanol was not given. Relative density source and purity not given; relative density $d=0.804$ (20 °C/4 °C).

Estimated Errors:
Nothing specified. The values given are the mean of three independent determinations.

Components:
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:
[14] S.V. Sidgwick and E.K. Embank, J. Chem. Soc. **1921,** 979.

Variables:
$t/°\text{C}=36.5–180.3$

Prepared by:
A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in 1-butanol

Temperature	Solubility	
$t/°\text{C}$	$100w_1$	$100x_1$ (compiler)
180.3	84.7	74.8
151.2	59.2	43.8
115.0	40.8	27.0
36.5	20.7	12.3

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and purification methods were described in [J. Walker and J.K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of 3-hydroxybenzoic acid was 201 °C.

1-Butanol was repeatedly fractionated, and distilled within 0.1 °C.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9]

(2) Ethane, 1,1-oxybis- (ethoxyethane, diethyl ether); $C_4H_{10}O$; [60-29-7]

Original Measurements:

[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).

Variables:

$t/°C=17.0$

Prepared by:

A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in diethyl ether at 17.0 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
97.3	0.704

[a]The solubility reported by the authors was expressed in grams per 100 cm^3 of acetone solution at 23 °C and in grams per 100 cm^3 of ether solution at 17 °C. The mass concentration, $\gamma_1=m_1/V$, was calculated by the compiler, where m_1 is the mass of component 1 and V is the total volume of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 20 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

No information was given.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9]

(2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

Original Measurements:

[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).

Variables:

$t/°C=23.0$

Prepared by:

A. Goto and H. Miyamoto

Solubility of 3-hydroxybenzoic acid in acetone at 23.0 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
260	1.88

[a]The solubility reported by the authors was expressed in grams per 100 cm^3 of acetone solution at 23 °C and in grams per 100 cm^3 of ether solution at 17 °C. The mass concentration, $\gamma_1=m_1/V$, was calculated by the compiler, where m_1 is the mass of component 1 and V is the total volume of the solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 20 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

No information was given.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9]

(2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

Original Measurements:

[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:

$t/°C=20.0$

Prepared by:

P. Scharlin

Solubility of 3-hydroxybenzoic acid in acetone at 20.0 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
207.2	1.500

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

3-Hydroxybenzoic acid was obtained from Shuchardt, reinst.

The source and purity of acetone were not given; relative density $d=0.791$ (20 °C/4 °C).

Estimated Errors:

Nothing specified. According to the author, the values given are the mean of three independent determinations.

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Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Ketones: 2-Butanone (butan-2-one, methyl ethyl ketone); C_4H_8O; [78-93-3] 2-Pentanone (pentan-2-one, methyl propyl ketone); $C_5H_{10}O$; [107-87-9]	[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=20.0$	P. Scharlin

Solubility of 3-hydroxybenzoic acid in ketones at 20.0 °C

	Solubility[a]	
Solvent	$\gamma_1/\mathrm{g\,dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\,dm^{-3}}$ (compiler)
2-Butanone	156.9	1.136
2-Pentanone	126.3	0.914

[a] In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

3-Hydroxybenzoic acid was obtained from Shuchardt, reinst.

The source and purity of 2-butanone and 2-pentanone were not given. Relative density *d* of 2-butanone and 2-pentanone are 0.805 (20 °C/4 °C) and 0.812 (15 °C/15 °C), respectively.

Estimated Errors:

Nothing specified. The values given are the mean of three independent determinations.

2.1.4.3. 4-Hydroxybenzoic acid

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) *n*-Heptane; C_7H_{16}; [142-82-5]	[14]N.V. Sidgwick and E.K. Ewbank, J. Chem. Soc. **1921**, 979.
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=197.0$ and 208.5	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in *n*-heptane

Temperature	Solubility	
$t/{}^\circ\mathrm{C}$	$100w_1$	$100x_1$ (compiler)
208.5(liq.)	1.80	1.31
197.0	1.06	0.771
208.5	Triple point	

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 14 for the salicylic acid–*n*-heptane system in Sec. 2.1.1.1.

Source and Purity of Materials:

The preparation and the purification of 4-hydroxybenzoic acid were described in [J. Walker and J.K. Wood, J. Chem. Soc. **117**, 40 (1920)]. Melting point of the purified acid was 213.0 °C.

n-Heptane was a specimen from *Pinus sabiniana*, which had been purified by treatment with sulfuric and nitric acids, and distillation.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[21]P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=25$	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in cyclohexane at 25 °C

Solubility	
pS	$10^3c_1/\mathrm{mol\,dm^{-3}}$ (compiler)
4.398	0.039 99

pS: The negative logarithm of the concentration in the saturated solution in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1. The acid was either of AnarR standard or recrystallized before use.

No information of the purity of cyclohexane was reported.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	[23]C.K. Hancock, J.N. Pawloski, and J.P. Idoux, J. Org. Chem. **31**, 3801 (1966).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=30$	A. Goto and H. Miyamoto

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Solubility of 4-hydroxybenzoic acid in cyclohexane at 30 °C

Solubility[a]	
$10^5 x_1$ (compiler)	$100 w_1$ (compiler)
3.70	6.08×10^{-3}

[a] In the original paper, the solubility was given as grams of acid per 100 g of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 23 for the 3-hydroxybenzoic acid–benzene system in Sec. 2.1.3.2.

Source and Purity of Materials:
The details are given in the compilation of Ref. 23 for the 3-hydroxybenzoic acid–benzene system in Sec. 2.1.3.2.

Estimated Errors:
Solubility (mole fraction units): The average deviation of the replicate values from the mean did not exceed 3%.
Temperature: Precision of ±0.02 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	[21] P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in chloroform at 25 °C.

Solubility	
pS	$10^3 c_1$/mol dm^{-3} (compiler)
2.991	1.021

pS: The negative logarithm of the concentration in the saturated solution in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:
The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	[19] A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

The solubility of 4-hydroxybenzoic acid in chloroform at 25 °C was reported as $10^4 x_1 = 1.5$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Methane, tetrachloro- (tetrachloromethane, carbon tetrachloride); CCl_4; [56-23-5]	[21] P.A. Ongley, J. Chem. Soc. **1954**, 3634.
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in carbon tetrachloride at 25 °C.

Solubility	
pS	$10^3 c_1$/mol dm^{-3} (compiler)
5.000	0.01000

pS: The negative logarithm of the concentration in the saturated solution in mol/l.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:
The details are given in the compilation of Ref. 21 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Ethane, 1,2-dichloro- (1,2-dichloroethane, ethylene dichloride); $C_2H_4Cl_2$; [107-06-2]	[19] A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

The solubility of 4-hydroxybenzoic acid in ethylene dichloride at 25 °C was reported as $10^4 x_1 = 1.1$.

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Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:
[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:
$t/°C=20.0$

Prepared by:
P. Scharlin

Solubility of 4-hydroxybenzoic acid in methanol at 20.0 °C

Solubility[a]	
γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
324.5	2.349

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
4-Hydroxybenzoic acid was obtained from Shuchardt, purity of 99.5%.
The source and purity of methanol was not given; relative density *d* =0.792 (20 °C/4 °C).

Estimated Errors:
Nothing specified. The value given is the mean of three independent determinations.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°C=25$

Prepared by:
A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in methanol at 25 °C

Molar volume of solvent	Solubility
v_2/cm^3 mol^{-1}	x_1
40.7	0.1142

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

Original Measurements:
[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:
$t/°C=20.0$

Prepared by:
P. Scharlin

Solubility of 4-hydroxybenzoic acid in 1-propanol at 20.0 °C

Solubility[a]	
γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
194.6	1.409

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
4-Hydroxybenzoic acid was obtained from Shuchardt, purity of 99.5%.
The source and purity of 1-propanol was not given; relative density *d* =0.804 (20 °C/4 °C).

Estimated Errors:
Nothing specified. The value given is the mean of three independent determinations.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

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Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in 1-propanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
75.1	0.1084

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in 1-pentanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
108.6	0.1145

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in 1-hexanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
125.2	0.1121

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in 1-octanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
158.4	0.1032

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 2-Propanol (propan-2-ol, isopropyl alcohol); C_3H_8O; [67-63-0]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

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Solubility of 4-hydroxybenzoic acid in 2-propanol at 25 °C

Molar volume of solvent	Solubility
v_2/cm^3 mol^{-1}	x_1
76.9	0.1297

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) 2-Methyl-1-propanol (2-methylpropan-1-ol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

t/°C=25

Prepared by:

A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in 2-methyl-1-propanol at 25 °C

Molar volume of solvent	Solubility
v_2/cm^3 mol^{-1}	x_1
92.4	0.0901

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) Benzyl alcohol (phenylmethanol); C_7H_8O; [100-51-6]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

t/°C=25

Prepared by:

A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in benzyl alcohol at 25 °C

Molar volume of solvent	Solubility
v_2/cm^3 mol^{-1}	x_1
103.9	0.0784

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) Diols and triols:

1,2-Ethanediol (ethane-1,2-diol, ethylene glycol); C_2H_6O; [107-21-1]

1,2-Propanediol (propane-1,2-diol, propylene glycol); $C_3H_8O_2$; [57-55-6]

1,2,3-Propanetriol (propane-1,2,3-triol, glycerol); $C_3H_8O_3$; [56-81-5]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

t/°C=25

Prepared by:

A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in diols and triols at 25 °C

	Molar volume of solvent	Solubility
Solvent	v_2/cm^3 mol^{-1}	x_1
Ethylene glycol	55.9	0.1132
Propylene glycol	73.7	0.1308
Glycerol	73.2	0.0301

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

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Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) Ethane, 1,1′-oxybis- (ethoxyethane, diethyl ether); $C_4H_{10}O$; [60-29-7]

Original Measurements:

[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).

Variables:

$t/°C=17$

Prepared by:

A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in diethyl ether at 17 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
94.3	0.683

[a]In the original paper, the solubility was given as grams per 100 cm^3 of acetone solution at 23 °C and in grams per 100 cm^3 of ether solution at 17 °C. The mass concentration, $\gamma_1=m_1/V$, was calculated by the compiler, where m_1 is the mass of component 1 and V is the total volume of the solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 20 for the salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

No information was given.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) Ethane, 1,1-oxybis- (ethoxyethane, diethyl ether); $C_4H_{10}O$; [60-29-7]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

$t/°C=25$

Prepared by:

A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in diethyl ether at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	10^2x_1
104.8	5.21

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

Original Measurements:

[20]J. Walker and J.K. Wood, J. Chem. Soc. Trans. **73**, 618 (1898).

Variables:

$t/°C=23$

Prepared by:

A. Goto and H. Miyamoto

Solubility of 4-hydroxybenzoic acid in acetone at 23 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
227	1.64

[a]In the original paper, the solubility was given as grams per 100 cm^3 of the acetone solution at 23 °C and in grams per 100 cm^3 of the ether solution at 17 °C. The mass concentration, $\gamma_1=m_1/V$, was calculated by the compiler, where m_1 is the mass of component 1 and V is the total volume of the solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 20 for the binary salicylic acid–benzene system in Sec. 2.1.3.1.

Source and Purity of Materials:

No information was given.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]

(2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

Original Measurements:

[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:

$t/°C=20$

Prepared by:

P. Scharlin

Solubility of 4-hydroxybenzoic acid in acetone at 20 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
205.5	1.488

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

4-Hydroxybenzoic acid was obtained from Shuchardt, purity of 99.5%.

Acetone: source and purity not given; relative density $d=0.791$ (20 °C/4 °C).

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Estimated Errors:

Nothing specified. The value given is the mean of three independent determinations.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

$t/°C=25$

Prepared by:

A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in acetone at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
74.0	0.1185

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 2-Butanone (butan-2-one, methyl ethyl ketone); C_4H_8O; [78-93-3]

Original Measurements:

[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:

$t/°C=20$

Prepared by:

P. Scharlin

Solubility of 4-hydroxybenzoic acid in 2-butanone at 20 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
205.8	1.490

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

4-Hydroxybenzoic acid was obtained from Shuchardt, purity of 99.5%.

2-Butanone; source and purity not given; relative density $d=0.805$ (20 °C/4 °C).

Estimated Errors:

Nothing specified. The value given is the mean of three independent determinations.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) 2-Pentanone (pentan-2-one, methyl propyl ketone); $C_5H_{10}O$; [107-87-9]

Original Measurements:

[15]E. Bergroth, Farm. Aikak. **70**, 91 (1961).

Variables:

$t/°C=20.0$

Prepared by:

P. Scharlin

Solubility of 4-hydroxybenzoic acid in 2-pentanone at 20.0 °C

Solubility[a]	
$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
170.9	1.237

[a]In the original paper, the solubility was given as grams per 100 ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 15 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

4-Hydroxybenzoic acid was obtained from Shuchardt, purity of 99.5%.

2-Pentanone: source and purity not given; relative density $d=0.812$ (15 °C/15 °C).

Estimated Errors:

Nothing specified. The value given is the mean of three independent determinations.

Components:

(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7]
(2) Carboxylic acids and their esters:
Acetic acid; $C_2H_4O_2$; [64-19-7]
Propionic acid; $C_3H_6O_2$; [79-09-4]
Ethyl acetate (ethyl acetate, acetic acid, ethyl ester); $C_4H_8O_2$; [141-78-6]
Butyl acetate (butyl acetate, acetic acid, butyl ester); $C_6H_{12}O_2$; [123-86-4]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

$t/°C=25$

Prepared by:

A. Goto and R. Goto

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Solubility of 4-hydroxybenzoic acid in acids and their esters at 25 °C

Solvent	Molar volume of solvent $v_2/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	Solubility 10^2x_1
Acetic acid	57.6	4.44
Propionic acid	75.0	3.47
Ethyl acetate	98.5	7.37
Butyl acetate	132.6	5.74

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Methane, 1,1′-sulfinyl-bis- (methylsulfinylmethane, dimethyl sulfoxide); C_2H_6OS; [67-68-5]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and R. Goto

The solubility of 4-hydroxybenzoic acid in dimethyl sulfoxide at 25 °C was reported as $x_1=0.3674$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Benzene, methyl- (toluene); C_7H_8; [108-88-3]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in toluene at 25 °C

Molar volume of solvent $v_2/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	Solubility $100x_1$
106.9	0.29×10^{-2}

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Acetophenone (1-phenylethanone, methyl phenyl ketone); C_8H_8O; [98-86-2]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in acetophenone at 25 °C

Molar volume of solvent $v_2/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	Solubility x_1
117.4	0.0223

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Estimated Errors:
Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Pyridine; C_5H_5N; [110-86-1]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and R. Goto

The solubility of 4-hydroxybenzoic acid in pyridine at 25 °C was reported as $x_1=0.1044$.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) 1,4-Dioxane (dioxane); $C_4H_8O_2$; [123-91-1]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of 4-hydroxybenzoic acid in dioxane at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm}^3\,\mathrm{mol}^{-1}$	10^2x_1
85.7	8.44

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Nothing specified.

2.1.5. Data for hydroxybenzoic acid–inorganic compound systems

2.1.5.1. Salicylic acid

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9]	[30]V.J. Krukonis and R.T. Kurnik, J. Chem. Eng. Data **30**, 247 (1985).
Variables:	**Prepared by:**
Pressure: $207-414\times10^5$ Pa $T/K=373.2$	H. Miyamoto and A. Goto

Solubility of salicylic acid in supercritical carbon dioxide at 373.2 K

Pressure[a]	Solubility
10^5 Pa	10^3x_1
207	2.07
276	2.99
345	3.53
414	6.99

[a] In the original paper, the pressure was given as bar. 1 bar$=10^5$ Pa.

Auxiliary Information

Methods/Apparatus/Procedure:

The solubility measurement was carried out in a flow system. For each solubility test, about 30 g of oven-dried, powdered solid was charged between layers of glass wool to an extraction vessel, and connected to the system. The experimental setup for measuring solubilities in supercritical carbon dioxide was mainly made up as follows: gas cylinder, compressor, surge tank, pressure gauge, extractor, heating tape, heated valve, U-tube, rotameter, and dry test meter (the experimental setup was shown in the paper). The glass wool served to keep the powder from compacting during passage of gas through the extractor. Carbon dioxide was supplied at about 87 bar pressure and 313 K to the suction side of a double-end diaphragm compressor and was compressed to the measurement pressure. The pressure was controlled by a back-pressure regulator which diverted the bulk of the compressed gas from the surge tank back to the suction side of the compressor, resulting in an almost pulse-free flow of gas to the extractor. The high-pressure gas passing downstream of the compressor was heated in a tube preheater to about 373 K and was passed through the extraction vessel, which was maintained at 373 ± 2 K by a temperature indicator/controller which measured the temperature via an iron-constantan thermocouple positioned in the bed of powder and which regulated power to a heater on the extractor. The solution (consisting of carbon dioxide and dissolved solid) leaving the extraction vessel was passed through a heated, flow-regulating, pressure let-down valve and expanded to ambient pressure. The solid dissolved by the gas passing though the extraction vessel precipitated during the pressure-reduction step and was separated from the gas in the U-tube collector whose exit junction was fitted with a glass wool filter to prevent fine solids from passing through the tube; a second U-tube with a more tightly packed glass wool filter was positioned downstream of the first collector and served to trap any fine particles that might have passed through the first filter. The ambient gas leaving the collection system passed through a rotameter for flow rate measurement and through a dry test meter for flow volume integration. The flow rate of the carbon dioxide through the extractor was maintained at 3 SLPM (standard liters per minute); that flow rate was found to ensure that solubility equilibrium was achieved in the gas at the exit of the extractor. Gravimetric determinations of the amount of solid collected coupled with the integrated volume of gas passing through the system during a solubility test allowed concentration levels of the solute in the gas to be calculated.

Source and Purity of Materials:

Salicylic acid was purchased from Aldrich Chem. Co. and the purity of the acid was more than 99%.

Carbon dioxide of grade 2.8 was purchased from Airco, Inc.

Estimated Errors:

Solubility: Precision of 1%.

Temperature: Precision of ±2 K.

Pressure: Nothing specified.

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Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7] (2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9]	[31]G.S. Gurdial and N.R. Foster, Ind. Eng. Chem. Res. **30**, 575 (1991).
Variables:	**Prepared by:**
Pressure: $81.1-202\times10^5$ Pa $t/°C=35-55$	H. Miyamoto and A. Goto

Solubility of salicylic acid in supercritical carbon dioxide

Pressure[a] 10^5 Pa	Temperature, $t/°C$			
	35	40	45	55
	Solubility, 10^4x_1			
81.1	0.34	0.11	0.07	—
86.1	0.75	0.18	—	—
91.2	1.23	0.66	0.17	—
96.2	—	0.97	—	—
101.3	1.64	1.36	0.83	0.34
111.4	1.86	1.63	1.27	0.73
121.6	2.08	1.92	1.72	1.3
131.7	2.21	2.23	2.27	2.28
141.8	—	2.53	2.59	2.68
152.0	2.41	2.76	3.05	3.34
162.1	—	3.02	3.25	4.01
172.2	2.62	3.15	3.59	4.81
182.4	2.80	3.5	3.85	5.46
192.5	—	3.64	—	5.72
202.6	3.06	3.95	4.32	6.24

[a] In the original paper, the pressure was given as bar. 1 bar$=10^5$ Pa.

Auxiliary Information

Methods/Apparatus/Procedure:

Equilibrium solubility data were obtained by using a continuous flow apparatus. Experimental setup was as follows: CO_2 cylinder, pressure gauge, shutoff valves, HPLC pump, temperature controller, surge tank, pressure transducer, equilibrium cell, Jerguson gauge, thermocouple, filter, regulating valve, collection tube, filter, saturator, wet test meter, and constant temperature bath (the experimental setup was shown in the paper). Liquid carbon dioxide was directed to a high-pressure liquid chromatography (HPLC) pump at ambient temperature after passing through a high-pressure 7 μm in-line filter. The HPLC pump was capable of delivering constant flow rates ranging from 0.1 to 9.9 ml/min at pressures up to 300 bar.

After compression, the carbon dioxide was charged into a 300 cm^3 sample cylinder that acted as a surge tank to dampen any pressure fluctuation. The high-pressure carbon dioxide then passed through a preheated coil, enabling the solvent to reach the desired extraction temperature. After reaching thermal equilibrium within the constant-temperature bath controlled to within ±0.5 °C, the solvent was introduced into a system of three high-pressure equilibrium cells connected in series. The first two equilibrium cells were 20 cm in length with an internal volume of 9.5 cm^3, while the third cell consisted of a high-pressure reflex Jerguson sight gauge. The sight gauge was considered important to ensure measurement of equilibrium solid solubility, since melting-point depression from interaction of high-pressure carbon dioxide with a solid has been observed [M.A. McHugh and T.J. Yogan, J. Chem. Eng. Data **29**, 112 (1984); H. Chang and D.G. Morrell, J. Chem. Eng. Data **30**, 74 (1985)]. The equilibrium cells were packed with the solute to be extracted with alternate layers of glass wool to prevent solid compaction. Glass wool was also plugged at the outlet of each column to avoid blockage of the lines connecting the extraction tubes. A 5 μm filter was installed after the last extraction cell to prevent entrainment of the solid during the experiment.

The system was maintained at the desired temperature and pressure for approximately 30 min before continuous operation commenced. The equilibrium temperature and pressure of the system were measured at the exit of the third equilibrium cell. The system pressure was measured with a Druck digital pressure transducer and indicator.

After achievement of equilibrium, the back-pressure regulating valve was opened slightly and the inlet flow rate was adjusted to maintain a constant system pressure. Upon expansion to ambient conditions, the dissolved solute precipitated out of the fluid phase. The precipitated solid was collected in a 2 μm filter, and the total flow of the gas was measured with a wet test meter at ambient conditions after bubbling through a saturator. To confirm that equilibrium solubility was being measured, measurements were made at various flow rates ranging from 200 to 400 cm^3/min (STP). Variation of the flow rate in this range was found to have no effect on the observed solubilities, thereby confirming that equilibrium solubility was being measured.

The determination of equilibrium solubility was achieved by a gravimetric method. At the end of each experiment, the mass of solid collected in the filter was determined with a Mettler balance. The back-pressure regulating valve and the transfer line were flushed with an organic solvent to recover all the precipitate.

Source and Purity of Materials:

Salicylic acid was purchased from Unilab, and the purity was more than 99%.

Liquid carbon dioxide was of food grade, and the minimum purity was 99.8%. All chemicals were used without further purification.

Estimated Errors:

Temperature: Precision of ±0.2 °C.

Pressure: Precision within ±0.5%.

2.1.5.2. 3-Hydroxybenzoic acid

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9]	[30]V.J. Krukonis and R.T. Kurnik, J. Chem. Eng. Data **30**, 247 (1985).
Variables:	**Prepared by:**
Pressure: $207-414\times10^5$ Pa $T/K=373.2$	H. Miyamoto and A. Goto

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Solubility of 3-hydroxybenzoic acid in supercritical carbon dioxide at 373.2 K

Pressure[a]	Solubility
10^5 Pa	$10^5 x_1$
207	2.71
276	5.35
345	7.54
414	11.2

[a] In the original paper, the pressure was given as bar. 1 bar=10^5 Pa.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 30 for the salicylic acid–carbon dioxide system in Sec. 2.1.5.1.

Source and Purity of Materials:

3-Hydroxybenzoic acid was purchased from Aldrich Chem. Co. and the purity of the acid was 99%.

Carbon dioxide of grade 2.8 was purchased from Airco, Inc.

Estimated Errors:

Solubility: Precision of 1%.

Temperature: Precision of ±2 K.

Pressure: Nothing specified.

2.1.5.3. 4-Hydroxybenzoic acid

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9]	[30] V.J. Krukonis and R.T. Kurnik, J. Chem. Eng. Data **30**, 247 (1985).
Variables:	**Prepared by:**
Pressure: 207–414×10^5 Pa T/K=373.2	H. Miyamoto and A. Goto

Solubility of 4-hydroxybenzoic acid in supercritical carbon dioxide at 373.2 K

Pressure[a]	Solubility
10^5 Pa	$10^5 x_1$
207	1.33
276	3.57
345	5.77
414	7.49

[a] In the original paper, the pressure was given as bar. 1 bar=10^5 Pa.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 30 for the salicylic acid–carbon dioxide system in Sec. 2.1.5.1.

Source and Purity of Materials:

4-Hydroxybenzoic acid was purchased from Aldrich Chem. Co. and the purity of the acid was more than 99%.

Carbon dioxide of grade 2.8 was purchased from Airco, Inc.

Estimated Errors:

Solubility: Precision of 1%.

Temperature: Precision of ±2 K.

Pressure: Nothing specified.

2.2. Paraben–organic compound systems

2.2.1. Critical evaluation of the solubility of parabens in alcohols

2.2.1.1. Methylparaben

Components:	Evaluators:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 22. Summary of experimental solubility data of methylparaben in methanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	39.5	12.1	Spectroscopy, Gravimetry	32
298.2	39.5	12.1	Spectroscopy	33
298.2		12.54	Spectroscopy	19
303.2	43.3	13.9	Spectroscopy	33
308.2	47.9	16.2	Spectroscopy	33
313.2	50.8	17.8	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: T/K=298.2–313.2

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data in Table 22 for the solubility of methylparaben in methanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3. The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 10, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.995

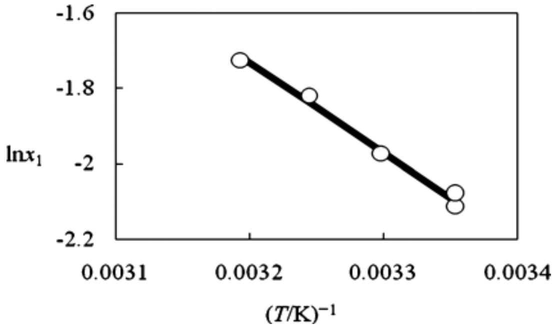

FIG. 10. Fitting curve of Eq. (2) and the observed data for methylparaben in methanol.

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Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-2392\pm 122$, $C=5.921\pm 0.401$

White circles in Fig. 10 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2392/T+5.921$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.995, as shown in Fig. 10. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 23 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 23. Observed data and recommended values calculated according to Eq. (2) for methylparaben in methanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	12.1	12.3
303.2	13.9	14.0
308.2	16.2	15.9
313.2	17.8	18.0

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/^\circ\mathrm{C}=25$

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in methanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.9166	39.5	0.121

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
Screw-capped bottles with the ester in excess and solvent were rotated for 24 h in a constant-temperature bath regulated at 25 °C. Samples were withdrawn through a pledget of glass wool into a pipet, which was wiped clean and allowed to drain into either a tared weighing bottle or a volumetric flask. Solubilities were determined by either a spectrophotometric or gravimetric procedure.

Source and Purity of Materials:
Methanol (Fisher certified) was used.

Methylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A. N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
$t/^\circ\mathrm{C}=25-40$

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in methanol

Temperature	Solubility	
$t/^\circ\mathrm{C}$	x_1	w_1[a] (compiler)
25	0.121	0.395
30	0.139	0.433
35	0.162	0.479
40	0.178	0.508

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The solute and solvent were placed in 15 ml vials attached to a submerged rotating plastic disk [A.N. Paruta, J. Pharm. Sci. **55**, 1208 (1966)]. After equilibration for 17 h at 25 °C, the sample of appropriate volume was withdrawn through a fine glass-wool plug fitted to a pipet with a short rubber tube. The sample solution was placed in a volumetric flask and diluted to the appropriate volume for analysis. The concentration of solute in solutions was determined spectrophotometrically. A Beckman DK-2 spectrophotometer was used to determine the absorbance of the solutions. The solubility of each solute was determined at least eight times for each solvent and average values were taken.

Source and Purity of Materials:
Spectrograde methylparaben was purchased from Matheson Coleman and Bell Co.

The source and the purity of methanol were not reported.

Estimated Errors:
Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/^\circ\mathrm{C}=25$

Prepared by:
A. Goto and R. Goto

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Solubility of methylparaben in methanol at 25 °C

Molar volume of solvent	Solubility
v_2/cm^3 mol^{-1}	x_1
40.7	0.1254

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

Methylparaben (Tenneco Chemical Inc.) was used as obtained. Melting point measured by a hot-stage method was 399.65 K.

The solvent was spectrophotometric grade, ACS grade, or redistilled before use.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$ [99-76-3]

(2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan
Rensuke Goto, University of Shizuoka, Shizuoka, Japan
Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 24. Summary of experimental solubility data of methylparaben in ethanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	36.0	14.7	Spectroscopy, Gravimetry	32
298.2	36.7	14.7	Spectroscopy	33
298.2		14.95	Spectroscopy	19
303.2	37.9	15.6	Spectroscopy	33
308.2	41.0	17.4	Spectroscopy	33
313.2	45.4	20.1	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: T/K=298.2–313.2

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of methylparaben in ethanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 24). The data points agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 11, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.980

Sample size: 6 data points

p-value (F test): 0.001

Constants: $A=-1804\pm183$, $C=4.126\pm0.602$

White circles in Fig. 11 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1804/T+4.126$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.980, as shown in Fig. 11. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

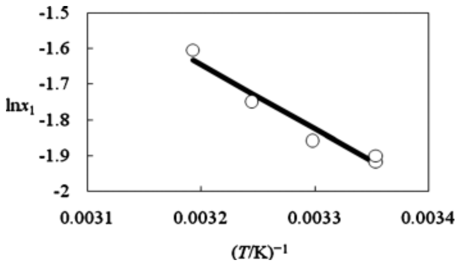

FIG. 11. Fitting curve of Eq. (2) and the observed data for methylparaben in ethanol.

Table 25 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 25. Observed data and recommended values calculated according to Eq. (2) for methylparaben in ethanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	14.7	14.6
303.2	15.6	16.2
308.2	17.4	17.8
313.2	20.1	19.5

Components:

(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]

(2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

Original Measurements:

[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:

t/°C=25

Prepared by:

A. Goto and R. Goto

Solubility of methylparaben in ethanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.8970	36.0	0.147

[a]In the original paper, the solubility was given as milligrams of the ester per grams of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

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Source and Purity of Materials:
Absolute ethanol was obtained from U.S. Industrial Chem. Co.
Methylparaben was obtained from Matheson, Coleman and Bell.
Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables: $t/°C=25-40$	**Prepared by:** A. Goto and R. Goto

Solubility of methylparaben in ethanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.147	0.367
30	0.156	0.379
35	0.174	0.410
40	0.201	0.454

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.
Source and Purity of Materials:
Spectrograde methylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.
Ethanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.
Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables: $t/°C=25$	**Prepared by:** A. Goto and R. Goto

Solubility of methylparaben in ethanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	x_1
58.7	0.1495

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.
Estimated Errors:
Solubility: The experimental variation was below 3%.
Temperature: Precision of ±0.2 °C.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 26. Summary of experimental solubility data of methylparaben in 1-propanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	29.5	13.8	Spectroscopy, Gravimetry	32
298.2	29.5	13.8	Spectroscopy	33
298.2		14.86	Spectroscopy	19
303.2	30.9	15.2	Spectroscopy	33
308.2	35.5	18.0	Spectroscopy	33
313.2	38.3	19.9	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of methylparaben in 1-propanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 26). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 12, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.975

Sample size: 6 data points

p-value (F test): 0.001

Constants: $A=-2146\pm 246$, $C=5.235\pm 0.812$

White circles in Fig. 12 represent the observed data and the black line corresponds to calculated values according to

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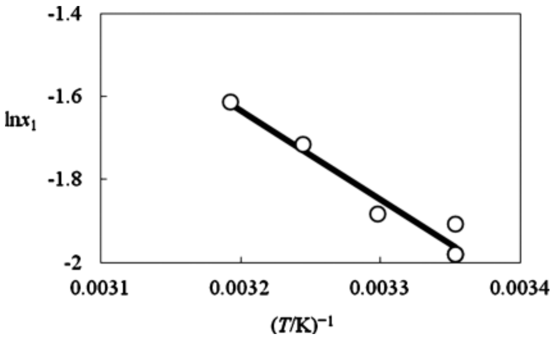

FIG. 12. Fitting curve of Eq. (2) and the observed data for methylparaben in 1-propanol.

Eq. (2) ($\ln x_1 = -2146/T + 5.235$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.975, as shown in Fig. 12. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 27 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 27. Observed data and recommended values calculated according to Eq. (2) for methylparaben in 1-propanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	13.8	14.0
303.2	15.2	15.8
308.2	18.0	17.7
313.2	19.9	19.8

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and R. Goto

Solubility of methylparaben in 1-propanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.8881	29.5	0.138

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Propanol (Baker analyzed) was used.

Methylparaben was obtained from Matheson, Coleman and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A. N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25-40$	A. Goto and R. Goto

Solubility of methylparaben in 1-propanol

Temperature	Solubility	
$t/°\mathrm{C}$	x_1	w_1[a] (compiler)
25	0.138	0.295
30	0.152	0.309
35	0.180	0.355
40	0.199	0.383

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde methylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature values.

1-Propanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

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Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in 1-propanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
75.1	0.1486

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Solubility: The experimental variation was below 3%.
Temperature: Precision of ±0.2 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Evaluators:
Ayako Goto, University of Shizuoka, Shizuoka, Japan
Rensuke Goto, University of Shizuoka, Shizuoka, Japan
Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 28. Summary of experimental solubility data of methylparaben in 1-butanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	26.2	14.6	Spectroscopy, Gravimetry	32
298.2	26.2	14.6	Spectroscopy	33
298.2		14.84	Spectroscopy	19
303.2	27.2	15.4	Spectroscopy	33
308.2	29.8	17.2	Spectroscopy	33
313.2	32.6	19.1	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of methylparaben in 1-butanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 28). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 13, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.986

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-1590\pm 135$, $C=3.405\pm 0.446$

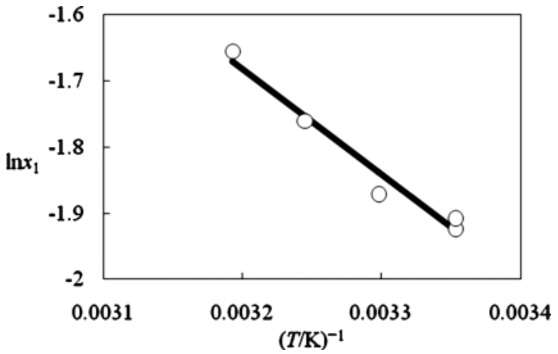

FIG. 13. Fitting curve of Eq. (2) and the observed data for methylparaben in 1-butanol.

White circles in Fig. 13 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1590/T+3.405$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.986, as shown in Fig. 13. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 29 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 29. Observed data and recommended values calculated according to Eq. (2) for methylparaben in 1-butanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	14.6	14.6
303.2	15.4	15.9
308.2	17.2	17.3
313.2	19.1	18.8

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in 1-butanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.8894	26.2	0.146

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

The source of 1-butanol was not reported.

Methyl 4-hydroxybenzoate was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°C=25-40$	A. Goto and R. Goto

Solubility of methylparaben in 1-butanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.146	0.262
30	0.154	0.272
35	0.172	0.298
40	0.191	0.326

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde methylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature values.

1-Butanol (TDY Mallinckrodt) was of analytical reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of methylparaben in 1-butanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm}^3\ \mathrm{mol}^{-1}$	x_1
92.0	0.1484

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 30. Summary of experimental solubility data of methylparaben in 1-hexanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	20.5	15.5	Spectroscopy, Gravimetry	32
298.2	20.5	15.5	Spectroscopy	33
298.2		14.77	Spectroscopy	19
303.2	21.2	16.6	Spectroscopy	33
308.2	25.3	18.6	Spectroscopy	33
313.2	26.2	20.5	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of methylparaben in 1-hexanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 30). The data points closely agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 14, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.989

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-1836\pm139$, $C=4.272\pm0.459$

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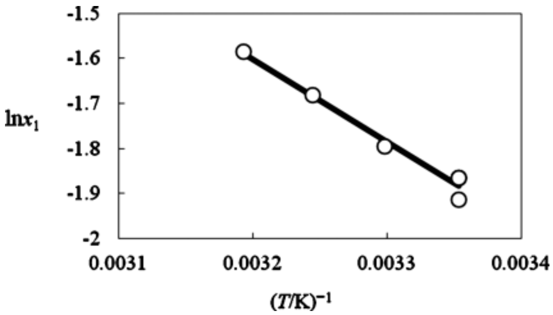

FIG. 14. Fitting curve of Eq. (2) and the observed data for methylparaben in 1-hexanol.

White circles in Fig. 14 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1 = -1836/T + 4.272$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.989, as shown in Fig. 14. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 31 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 31. Observed data and recommended values calculated according to Eq. (2) for methylparaben in 1-hexanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	15.5	15.2
303.2	16.6	16.8
308.2	18.6	18.6
313.2	20.5	20.4

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/°C = 25$

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in 1-hexanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.8712	20.5	0.155

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
1-Hexanol (Eastman-Kodak No. 50) was used.
Methylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
$t/°C = 25–40$

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in 1-hexanol

Temperature	Solubility	
t/°C	x_1	w_1[a] (compiler)
25	0.155	0.205
30	0.166	0.212
35	0.186	0.253
40	0.205	0.262

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde methylparaben was purchased from Matheson Coleman and Bell Co. Melting points were within 1 °C of literature values.
The purity of 1-hexanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°C = 25$

Prepared by:
A. Goto and R. Goto

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Solubility of methylparaben in 1-hexanol at 25 °C

Molar volume of solvent	Solubility
v_2/cm^3 mol^{-1}	x_1
125.2	0.1477

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 32. Summary of experimental solubility data of methylparaben in 1-decanol

T/K	100w_1	100x_1	Analytical method	Reference
298.2	9.0	8.8	Spectroscopy, Gravimetry	32
298.2	8.8	8.8	Spectroscopy	33
303.2	10.3	10.9	Spectroscopy	33
308.2	12.2	12.8	Spectroscopy	33
313.2	13.9	14.4	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in n-heptane.

The number of publications: 2

The range of temperature: T/K=298.2–313.2

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of methylparaben in 1-decanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 32). The data points closely agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 15, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.995

Sample size: 5 data points

p-value (F test): 0.000

Constants: $A=-3136\pm189$, $C=8.100\pm0.622$

White circles in Fig. 15 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-3136/T+8.100$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.995, as shown in Fig. 15. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

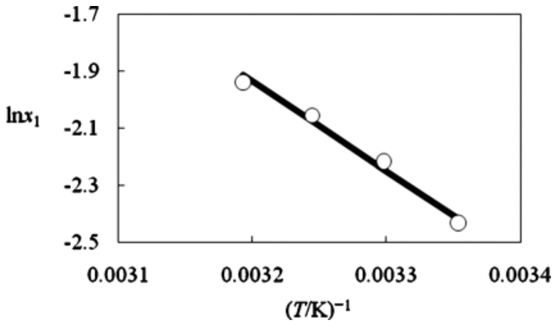

FIG. 15. Fitting curve of Eq. (2) and the observed data for methylparaben in 1-decanol.

Table 33 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 33. Observed data and recommended values calculated according to Eq. (2) for methylparaben in 1-decanol

T/K	100x_1(obs)	100x_1(rec)
298.2	8.8	8.9
303.2	8.8	10.6
308.2	10.9	12.5
313.2	12.8	14.8

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
t/°C=25	A. Goto and R. Goto

Solubility of methylparaben in 1-decanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	100w_1[a] (compiler)	x_1
0.8658	9.0	0.088

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

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Source and Purity of Materials:

The source of 1-decanol was not reported.

Methylparaben was obtained from Matheson, Coleman and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°C=25-40$	A. Goto and R. Goto

Solubility of methylparaben in 1-decanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.088	0.088
30	0.109	0.103
35	0.128	0.122
40	0.144	0.139

[a] In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde methylparaben was purchased from Matheson Coleman and Bell Co. Melting points were within 1 °C of literature values.

The purity of 1-decanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

2.2.1.2. Ethylparaben

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

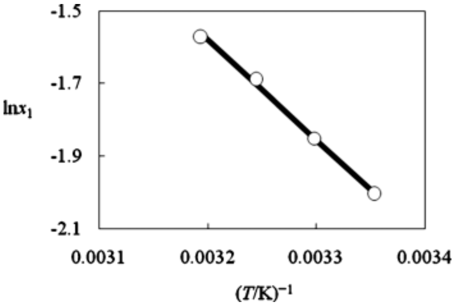

FIG. 16. Fitting curve of Eq. (2) and the observed data for ethylparaben in methanol.

Critical Evaluation

TABLE 34. Summary of experimental solubility data of ethylparaben in methanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	45.2	13.5	Spectroscopy, Gravimetry	32
298.2	45.2	13.5	Spectroscopy	33
303.2	49.0	15.7	Spectroscopy	33
308.2	54.1	18.5	Spectroscopy	33
313.2	57.0	20.8	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of ethylparaben in methanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 34). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 16, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.999

Sample size: 5 data points

p-value (F test): 0.000

Constants: $A=-2740\pm75$, $C=7.188\pm0.248$

White circles in Fig. 16 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2740/T+7.188$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.999, as shown in Fig. 16. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 35 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

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TABLE 35. Observed data and recommended values calculated according to Eq. (2) for ethylparaben in methanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	13.5	13.5
303.2	15.7	15.7
308.2	18.5	18.2
313.2	20.8	21.0

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of ethylparaben in methanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.9256	45.2	0.135

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Methanol (Fisher certified) was used.

Ethylparaben was obtained from Matheson, Coleman and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°C=25-40$	A. Goto and R. Goto

Solubility of ethylparaben in methanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.135	0.452
30	0.157	0.490
35	0.185	0.541
40	0.208	0.576

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde ethylparaben was purchased from Matheson Coleman and Bell Co.

The source and the purity of methanol were not reported.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	Evaluators:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 36. Summary of experimental solubility data of ethylparaben in ethanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	41.2	16.5	Spectroscopy, Gravimetry	32
298.2	41.2	16.5	Spectroscopy	33
303.2	44.9	18.4	Spectroscopy	33
308.2	50.1	21.8	Spectroscopy	33
313.2	50.5	22.0	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in n-heptane.

The number of publications: 2

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of ethylparaben in ethanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 36). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 17, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.971

Sample size: 5 data points

p-value (F test): 0.006

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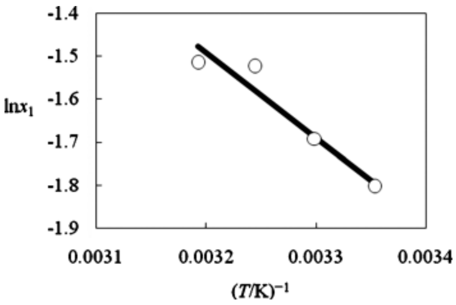

FIG. 17. Fitting curve of Eq. (2) and the observed data for ethylparaben in ethanol.

Constants: $A=-1974\pm282$, $C=4.823\pm0.929$

White circles in Fig. 17 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1974/T+4.823$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.971, as shown in Fig. 17. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 37 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 37. Observed data and recommended values calculated according to Eq. (2) for ethylparaben in ethanol

T/K	100x_1(obs)	100x_1(rec)
298.2	16.5	16.6
303.2	18.4	18.5
308.2	21.8	20.6
313.2	22.0	22.8

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of ethylparaben in ethanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	100w_1[a] (compiler)	x_1
0.9098	41.2	0.165

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Absolute ethanol was obtained from U.S. Industrial Chemical Co.

Ethylparaben was obtained from Matheson, Coleman and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°C=25-40$	A. Goto and R. Goto

Solubility of ethylparaben in ethanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.165	0.412
30	0.184	0.449
35	0.218	0.501
40	0.220	0.505

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde ethylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature values.

Ethanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

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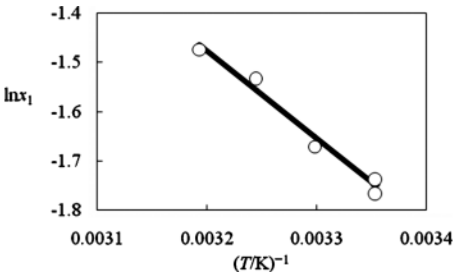

FIG. 18. Fitting curve of Eq. (2) and the observed data for ethylparaben in 1-propanol.

Critical Evaluation

TABLE 38. Summary of experimental solubility data of ethylparaben in 1-propanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	36.3	17.1	Gravimetry, Spectroscopy	34
298.2	36.2	17.6	Spectroscopy, Gravimetry	32
298.2	36.2	17.6	Spectroscopy	33
303.2	38.8	18.8	Spectroscopy	33
308.2	42.9	21.6	Spectroscopy	33
313.2	44.7	22.9	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of ethylparaben in 1-propanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 38). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 18, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.989

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-1768\pm133$, $C=4.180\pm0.439$

White circles in Fig. 18 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1768/T+4.180$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.989, as shown in Fig. 18. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 39 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 39. Observed data and recommended values calculated according to Eq. (2) for ethylparaben in 1-propanol

T/K	$100x_1(\mathrm{obs})$	$100x_1(\mathrm{rec})$
298.2	17.6	17.4
303.2	18.8	19.2
308.2	21.6	21.1
313.2	22.9	23.1

Components: (1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	**Original Measurements:** [34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables: $t/^\circ\mathrm{C}=25$	**Prepared by:** A. Goto and R. Goto

Solubility of ethylparaben in 1-propanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	w_1[a] (compiler)	x_1
0.9079	0.3626	0.171

[a] In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

A slight excess of the ester was added to approximately 40 ml of solvent in a screw-top bottle. A closure was made with aluminum foil, the top fixed tightly over the foil, and the whole sealed with several turns of electrical tape. The bottles were shaken in a constant-temperature bath for 24 h. The equilibrated solutions were removed and filtered. The analysis was carried out gravimetrically and spectrophotometrically.

Source and Purity of Materials:

Fisher certified grade 1-propanol (b.p. 96.9–97.2 °C) was used without further purification.

Estimated Errors:

Solubility: Nothing specified.

Temperature: ±0.05 °C.

Components: (1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	**Original Measurements:** [32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables: $t/^\circ\mathrm{C}=25$	**Prepared by:** A. Goto and R. Goto

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Solubility of ethylparaben in 1-propanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.9081	36.2	0.176

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Propanol (Baker analyzed) was used.

Ethylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]

(2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

Original Measurements:

[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:

t/°C=25–40

Prepared by:

A. Goto and R. Goto

Solubility of ethylparaben in 1-propanol

Temperature	Solubility	
t/°C	x_1	w_1[a] (compiler)
25	0.176	0.362
30	0.188	0.388
35	0.216	0.429
40	0.229	0.447

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde ethylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature value.

1-Propanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

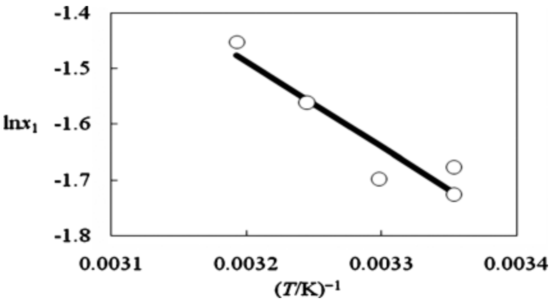

FIG. 19. Fitting curve of Eq. (2) and the observed data for ethylparaben in 1-butanol.

Components:

(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]

(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan

Rensuke Goto, University of Shizuoka, Shizuoka, Japan

Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 40. Summary of experimental solubility data of ethylparaben in 1-butanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	34.0	18.7	Gravimetry, Spectroscopy	34
298.2	34.0	17.8	Spectroscopy, Gravimetry	32
298.2	34.0	17.8	Spectroscopy	33
303.2	33.5	18.3	Spectroscopy	33
308.2	37.3	21.0	Spectroscopy	33
313.2	40.7	23.4	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in n-heptane.

The number of publications: 3

The range of temperature: T/K=298.2–313.2

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of ethylparaben in 1-butanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 40). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 19, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.946

Sample size: 6 data points

p-value (F test): 0.004

Constants: $A=-1537\pm263$, $C=3.431\pm0.867$

White circles in Fig. 19 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1537/T+3.431$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.946, as shown in Fig. 19. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

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Table 41 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 41. Observed data and recommended values calculated according to Eq. (2) for ethylparaben in 1-butanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	18.7	17.8
303.2	18.3	19.4
308.2	21.0	21.1
313.2	23.4	22.8

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:
[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of ethylparaben in 1-butanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	w_1[a] (compiler)	x_1
0.9071	0.3398	0.187

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
Fisher certified grade 1-butanol (b.p. 116.6–117.8 °C) was used without further purification.
The ester (purified grade) was recrystallized from chloroform until a sharp melting point was reached.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of ethylparaben in 1-butanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$ (compiler)	x_1[a]
0.9082	34.0	0.178

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
The source and the purity of 1-butanol were not reported.
Ethylparaben was obtained from Matheson, Coleman and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
$t/°C=25–40$

Prepared by:
A. Goto and R. Goto

Solubility of ethylparaben in 1-butanol

Temperature	Solubility	
t/°C	x_1	w_1[a] (compiler)
25	0.178	0.340
30	0.183	0.335
35	0.210	0.373
40	0.234	0.407

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde ethylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature value.
1-Butanol (TDY Mallinckrodt) was of analytical reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of ±0.1 °C.

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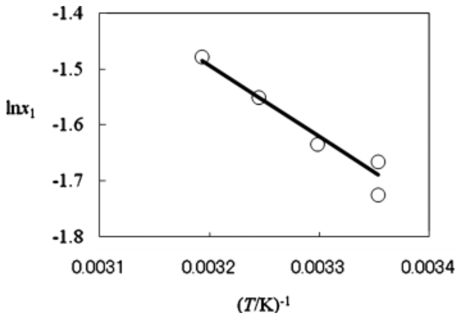

FIG. 20. Fitting curve of Eq. (2) and the observed data for ethylparaben in 1-hexanol.

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Evaluators:
Ayako Goto, University of Shizuoka, Shizuoka, Japan
Rensuke Goto, University of Shizuoka, Shizuoka, Japan
Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 42. Summary of experimental solubility data of ethylparaben in 1-hexanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	26.0	17.8	Gravimetry, Spectroscopy	34
298.2	26.0	18.9	Spectroscopy, Gravimetry	32
298.2	26.0	18.9	Spectroscopy	33
303.2	28.2	19.5	Spectroscopy	33
308.2	30.5	21.2	Spectroscopy	33
313.2	32.5	22.8	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of ethylparaben in 1-hexanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 42). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 20, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.966

Sample size: 6 data points

p-value (F test): 0.002

Constants: $A=-1278\pm172$, $C=2.595\pm0.566$

White circles in Fig. 20 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1278/T+2.595$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.966, as shown in Fig. 20. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 43 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 43. Observed data and recommended values calculated according to Eq. (2) for ethylparaben in 1-hexanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	17.8	18.5
303.2	19.5	19.8
308.2	21.2	21.2
313.2	22.8	22.7

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

Variables:
$t/^\circ\mathrm{C}=25$

Prepared by:
A. Goto and R. Goto

Solubility of ethylparaben in 1-hexanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	w_1[a] (compiler)	x_1
0.8888	0.2604	0.178

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
1-Hexanol (b.p. 156.5–157.5 °C) obtained from Eastman Organic Chemicals was redistilled.
The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/^\circ\mathrm{C}=25$

Prepared by:
A. Goto and R. Goto

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Solubility of ethylparaben in 1-hexanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.8860	26.0	0.189

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Hexanol (Eastman-Kodak No. 50) was used.

Ethylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]

(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:

[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:

t/°C=25–40

Prepared by:

A. Goto and R. Goto

Solubility of ethylparaben in 1-hexanol

Temperature	Solubility	
t/°C	x_1	w_1[a] (compiler)
25	0.189	0.260
30	0.195	0.282
35	0.212	0.305
40	0.228	0.325

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde ethylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of the literature value.

The purity of 1-hexanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

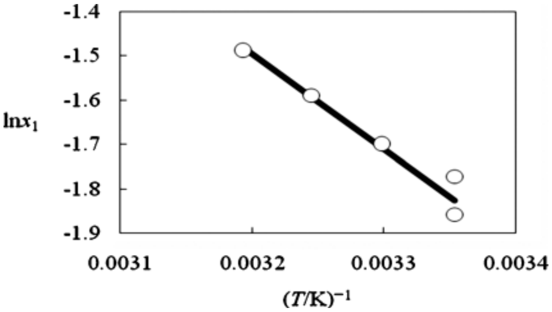

FIG. 21. Fitting curve of Eq. (2) and the observed data for ethylparaben in 1-octanol.

Components:

(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]

(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan

Rensuke Goto, University of Shizuoka, Shizuoka, Japan

Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 44. Summary of experimental solubility data of ethylparaben in 1-octanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	20.7	17.0	Gravimetry, Spectroscopy	34
298.2	20.7	15.6	Spectroscopy, Gravimetry	32
298.2	20.7	15.6	Spectroscopy	33
303.2	22.2	18.3	Spectroscopy	33
303.2		15.0	Spectroscopy	35
308.2	24.6	20.4	Spectroscopy	33
313.2	27.1	22.6	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 4

The range of temperature: T/K=298.2–313.2

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of ethylparaben in 1-octanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 44). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 21, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.977

Sample size: 6 data points (the datum from Ref. 35 of Table 44 was deleted because the multiple correlation coefficient was shown to be 0.865)

p-value (F test): 0.001

Constants: $A=-2149\pm234$, $C=5.380\pm0.773$

White circles in Fig. 21 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2149/T+5.380$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of

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0.977, as shown in Fig. 21. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 45 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 45. Observed data and recommended values calculated according to Eq. (2) for ethylparaben in 1-octanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	17.0	16.1
303.2	18.3	18.1
308.2	20.4	20.3
313.2	22.6	22.7

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

Variables:
t/ °C=25

Prepared by:
A. Goto and R. Goto

Solubility of ethylparaben in 1-octanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	w_1[a] (compiler)	x_1
0.8780	0.2065	0.170

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
1-Octanol (b.p. 194–195 °C) obtained from Eastman Organic Chemicals was redistilled.
The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
t/ °C=25

Prepared by:
A. Goto and R. Goto

Solubility of ethylparaben in 1-octanol at 25 °C

Density	Solubility[a]	
ρ/g cm^{-3}	$100w_1$ (compiler)	x_1
0.8791	20.7	0.156

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
1-Octanol (Eastman-Kodak No. 50) was used.
Ethylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
t/ °C=25–40

Prepared by:
A. Goto and R. Goto

Solubility of ethylparaben in 1-octanol

Temperature	Solubility[a]	
t/ °C	x_1	w_1 (compiler)
25	0.156	0.207
30	0.183	0.222
35	0.204	0.246
40	0.226	0.271

[a]In the original paper, the solubility was given as mg/g of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde ethylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature values.

The purity of 1-octanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[35]S.H. Yalkowsky, S.C. Valvani, and T.J. Roseman, J. Pharm. Sci. **72**, 866 (1983).
Variables:	**Prepared by:**
$t/°C=30$	A. Goto and R. Goto

Solubility of ethylparaben in 1-octanol at 30 °C

Solubility	
$\log_{10} x_1$	x_1 (compiler)
−0.83	0.15

Auxiliary Information

Methods/Apparatus/Procedure:

An excess amount of solute was allowed to equilibrate with water in a sealed vial for 24 h at 30 °C. After equilibration, the samples were filtered through either a 0.22 μm porous or a 1.2 μm silver membrane filter which was preequilibrated at 30 °C. Analysis of the filtrate was performed using UV spectrophotometry.

Source and Purity of Materials:

Purest grade ethylparaben was obtained from commercial sources (Aldrich, Eastman, and Fluka), and was used as received.

Reagent-grade octanol was obtained from Aldrich.

Estimated Errors:

Nothing specified.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

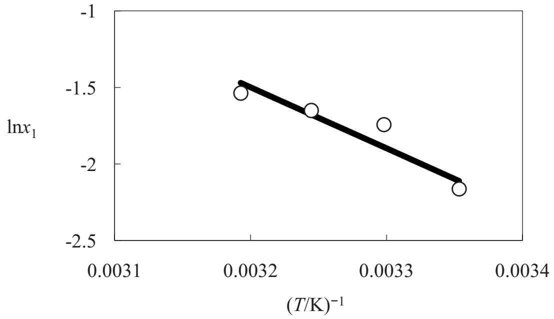

FIG. 22. Fitting curve of Eq. (2) and the observed data for ethylparaben in 1-decanol.

Critical Evaluation

TABLE 46. Summary of experimental solubility data of ethylparaben in 1-decanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	14.8	11.5	Spectroscopy, Gravimetry	32
298.2	14.8	11.5	Spectroscopy	33
303.2	18.2	17.5	Spectroscopy	33
308.2	20.0	19.2	Spectroscopy	33
313.2	22.3	21.5	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of ethylparaben in 1-decanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 46). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 22, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.952

Sample size: 5 data points

p-value (F test): 0.013

Constants: $A=-3993\pm741$, $C=11.28\pm2.44$

White circles in Fig. 22 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-3993/T+11.28$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.952, as shown in Fig. 22. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 47 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

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TABLE 47. Observed data and recommended values calculated according to Eq. (2) for ethylparaben in 1-decanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	11.5	12.1
303.2	17.5	15.1
308.2	19.2	18.7
313.2	21.5	23.0

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of ethylparaben in 1-decanol at 25 °C

Density	Solubility[a]	
ρ/g cm^{-3}	$100w_1$ (compiler)	x_1
0.8702	14.8	0.115

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
The source of 1-decanol was not reported.

Ethylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°C=25-40$	A. Goto and R. Goto

Solubility of ethylparaben in 1-decanol

Temperature	Solubility	
t/°C	x_1	w_1[a] (compiler)
25	0.115	0.148
30	0.175	0.182
35	0.192	0.200
40	0.215	0.223

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde ethylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of the literature value.

The purity of 1-decanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:
Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

2.2.1.3. Propylparaben

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 48. Summary of experimental solubility data of propylparaben in methanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	54.0	17.2	Spectroscopy, Gravimetry	32
298.2	54.0	17.2	Spectroscopy	33
303.2	59.5	20.7	Spectroscopy	33
308.2	63.9	24.0	Spectroscopy	33
313.2	68.2	27.6	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in n-heptane.

The number of publications: 2

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of propylparaben in methanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 48). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 23, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

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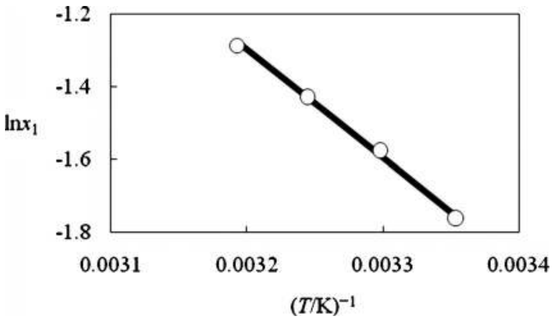

FIG. 23. Fitting curve of Eq. (2) and the observed data for propylparaben in methanol.

Multiple correlation coefficient: 0.999

Sample size: 5 data points

p-value (F test): 0.000

Constants: $A=-2962\pm 84$, $C=8.179\pm 0.275$

White circles in Fig. 23 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2962/T+8.179$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.999, as shown in Fig. 23. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 49 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 49. Observed data and recommended values calculated according to Eq. (2) for propylparaben in methanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	17.2	17.3
303.2	20.7	20.4
308.2	24.0	23.9
313.2	27.6	27.8

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
t/°C=25	A. Goto and R. Goto

Solubility of propylparaben in methanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.9318	54.0	0.172

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Methanol (Fisher certified) was used.

Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
t/°C=25–40	A. Goto and R. Goto

Solubility of propylparaben in methanol

Temperature	Solubility	
t/°C	x_1	w_1[a] (compiler)
25	0.172	0.540
30	0.207	0.595
35	0.240	0.639
40	0.276	0.682

[a] In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde propylparaben was purchased from Matheson Coleman and Bell Co.

The source and the purity of methanol were not reported.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

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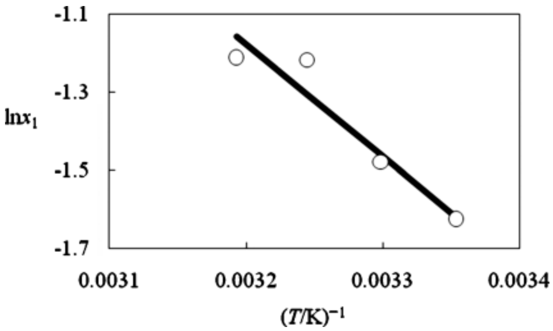

FIG. 24. Fitting curve of Eq. (2) and the observed data for propylparaben in ethanol.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 50. Summary of experimental solubility data of propylparaben in ethanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	49.0	19.7	Spectroscopy, Gravimetry	32
298.2	49.0	19.7	Spectroscopy	33
303.2	53.5	22.8	Spectroscopy	33
308.2	62.1	29.6	Spectroscopy	33
313.2	62.4	29.8	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of propylparaben in ethanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 50). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 24, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.935

Sample size: 5 data points

p-value (F test): 0.007

Constants: $A=-2859\pm 435$, $C=7.970\pm 1.430$

White circles in Fig. 24 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2859/T+7.970$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.935, as shown in Fig. 24. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 51 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 51. Observed data and recommended values calculated according to Eq. (2) for propylparaben in ethanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	19.7	19.8
303.2	22.8	23.2
308.2	29.6	27.1
313.2	29.8	31.4

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25$	A. Goto and R. Goto

Solubility of propylparaben in ethanol at 25 °C

Density	Solubility[a]	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.9076	49.0	0.197

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Absolute ethanol was obtained from U.S. Industrial Chemical Co.

Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°\mathrm{C}=25-40$	A. Goto and R. Goto

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Solubility of propylparaben in ethanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.197	0.490
30	0.228	0.535
35	0.296	0.621
40	0.298	0.624

[a] In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde propylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature value.

Ethanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 52. Summary of experimental solubility data of propylparaben in 1-propanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	43.6	20.5	Spectroscopy, Gravimetry	34
298.2	43.6	19.8	Spectroscopy, Gravimetry	32
298.2	43.6	19.8	Spectroscopy	33
303.2	47.8	23.6	Spectroscopy	33
308.2	52.7	27.3	Spectroscopy	33
313.2	55.7	29.8	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of propylparaben in 1-propanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 52). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 25, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

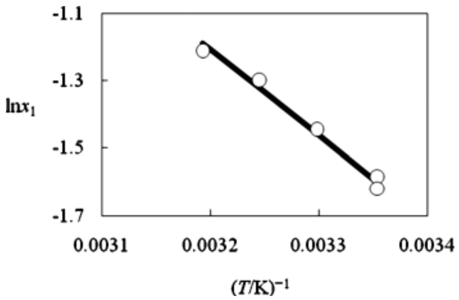

FIG. 25. Fitting curve of Eq. (2) and the observed data for propylparaben in 1-propanol.

Multiple correlation coefficient: 0.993

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-2571\pm154$, $C=7.019\pm0.509$

White circles in Fig. 25 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2571/T+7.019$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.993, as shown in Fig. 25. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 53 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 53. Observed data and recommended values calculated according to Eq. (2) for propylparaben in 1-propanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	20.5	20.2
303.2	23.6	23.2
308.2	27.3	26.7
313.2	29.8	30.5

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[34] F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

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Solubility of propylparaben in 1-propanol at 25 °C

Density	Solubility	
ρ/ g cm^{-3}	w_1[a] (compiler)	x_1
0.9204	0.4363	0.205

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

Fisher certified grade 1-propanol (b.p. 96.9–97.2 °C) was used without further purification.

The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:

Solubility: Nothing specified.

Temperature: ±0.05 °C.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
t/ °C=25	A. Goto and R. Goto

Solubility of propylparaben in 1-propanol at 25 °C

Density	Solubility	
ρ/ g cm^{-3}	100w_1[a] (compiler)	x_1
0.9112	43.6	0.198

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Propanol (Baker analyzed) was used.

Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
t/ °C=25–40	A. Goto and R. Goto

Solubility of propylparaben in 1-propanol

Temperature	Solubility	
t/ °C	x_1	w_1[a] (compiler)
25	0.198	0.436
30	0.236	0.478
35	0.273	0.527
40	0.298	0.557

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde propylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of the literature value.

1-Propanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	Evaluators:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 54. Summary of experimental solubility data of propylparaben in 1-butanol

T/K	100w_1	100x_1	Analytical method	Reference
298.2	39.4	21.1	Spectroscopy, Gravimetry	34
298.2	39.4	20.6	Spectroscopy, Gravimetry	32
298.2	39.4	20.6	Spectroscopy	33
303.2	44.1	24.5	Spectroscopy	33
308.2	48.4	27.8	Spectroscopy	33
313.2	52.8	31.6	Spectroscopy	33

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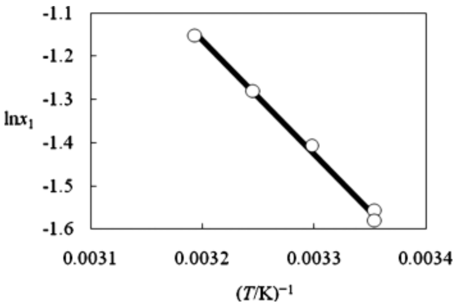

FIG. 26. Fitting curve of Eq. (2) and the observed data for propylparaben in 1-butanol.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of propylparaben in 1-butanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 54). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 26, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.998

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-2633\pm89$, $C=7.260\pm0.293$

White circles in Fig. 26 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2633/T+7.260$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.998, as shown in Fig. 26. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 55 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 55. Observed data and recommended values calculated according to Eq. (2) for propylparaben in 1-butanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	21.1	20.8
303.2	24.5	24.1
308.2	27.8	27.8
313.2	31.6	31.8

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=25$	A. Goto and R. Goto

Solubility of propylparaben in 1-butanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	w_1[a] (compiler)	x_1
0.9146	0.3940	0.211

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

Fisher certified grade 1-butanol (b.p. 116.6–117.8 °C) was used without further purification.

The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:

Solubility: Nothing specified.

Temperature: ±0.05 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=25$	A. Goto and R. Goto

Solubility of propylparaben in 1-butanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.9066	39.4	0.206

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

The source of 1-butanol was not reported.

Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3]

(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:

[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:

$t/°C=25-40$

Prepared by:

A. Goto and R. Goto

Solubility of propylparaben in 1-butanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.206	0.394
30	0.245	0.441
35	0.278	0.484
40	0.316	0.528

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde propylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

1-Butanol (TDY Mallinckrodt) was of analytical reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3]

(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan

Rensuke Goto, University of Shizuoka, Shizuoka, Japan

Hiroshi Fukuda, Kitasato University, Tokyo, Japan

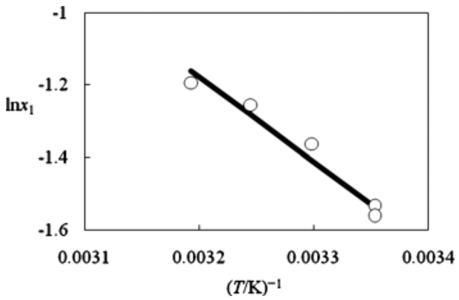

FIG. 27. Fitting curve of Eq. (2) and the observed data for propylparaben in 1-hexanol.

Critical Evaluation

TABLE 56. Summary of experimental solubility data of propylparaben in 1-hexanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	32.7	21.6	Spectroscopy, Gravimetry	34
298.2	32.6	21.0	Spectroscopy, Gravimetry	32
298.2	32.6	21.0	Spectroscopy	33
303.2	36.2	25.6	Spectroscopy	33
308.2	41.2	28.5	Spectroscopy	33
313.2	43.4	30.3	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of propylparaben in 1-hexanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 56). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 27, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.981

Sample size: 6 data points

p-value (F test): 0.001

Constants: $A=-2355\pm 232$, $C=6.360\pm 0.765$

White circles in Fig. 27 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2355/T+6.360$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.981, as shown in Fig. 27. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 57 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

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TABLE 57. Observed data and recommended values calculated according to Eq. (2) for propylparaben in 1-hexanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	21.6	21.5
303.2	25.6	24.5
308.2	28.5	27.7
313.2	30.3	31.3

Components:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

Variables:
t/°C=25

Prepared by:
A. Goto and R. Goto

Solubility of propylparaben in 1-hexanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	w_1[a] (compiler)	x_1
0.8992	0.3265	0.216

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
1-Hexanol (b.p. 156.5–157.5 °C) obtained from Eastman Organic Chemicals was redistilled.

The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
t/°C=25

Prepared by:
A. Goto and R. Goto

Solubility of propylparaben in 1-hexanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.8981	32.6	0.210

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
1-Hexanol (Eastman-Kodak No. 50) was used.

Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
t/°C=25–40

Prepared by:
A. Goto and R. Goto

Solubility of propylparaben in 1-hexanol

Temperature	Solubility	
t/°C	x_1	w_1[a] (compiler)
25	0.210	0.326
30	0.256	0.362
35	0.285	0.412
40	0.303	0.434

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde propylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

The purity of 1-hexanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of ±0.1 °C.

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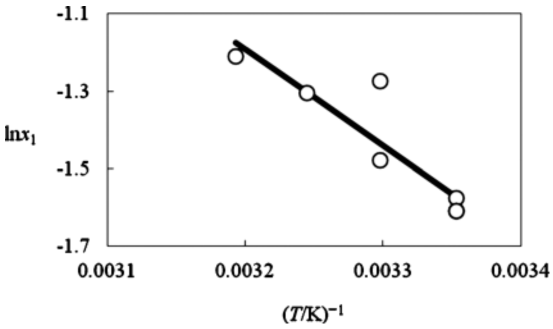

FIG. 28. Fitting curve of Eq. (2) and the observed data for propylparaben in 1-octanol.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 58. Summary of experimental solubility data of propylparaben in 1-octanol

T/K	c_1/mol dm^{-3}	100w_1	100x_1	Analytical method	Reference
298.2		26.6	20.7	Spectroscopy, Gravimetry	34
298.2		26.6	20.0	Spectroscopy, Gravimetry	32
298.2		26.6	20.0	Spectroscopy	33
298.2	2.39			Spectroscopy	36
303.2		29.0	22.8	Spectroscopy	33
303.2			28.0	Spectroscopy	35
308.2		33.9	27.1	Spectroscopy	33
313.2		37.0	29.8	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 5

The range of temperature: T/K = 298.2–313.2

The units: molar concentration, mass percent, and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of propylparaben in 1-octanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 58). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 28, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.903

Sample size: 7 data points

p-value (F test): 0.005

Constants: $A = -2490 \pm 529$, $C = 6.777 \pm 1.744$

White circles in Fig. 28 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1 = -2490/T + 6.777$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.903, as shown in Fig. 28. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 59 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 59. Observed data and recommended values calculated according to Eq. (2) for propylparaben in 1-octanol

T/K	100x_1(obs)	100x_1(rec)
298.2	20.7	20.7
303.2	22.8	23.8
308.2	27.1	27.2
313.2	29.8	30.9

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared By:**
t/°C = 25	A. Goto and R. Goto

Solubility of propylparaben in 1-octanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	w_1[a]	x_1
0.8869	0.2655	0.207

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

1-Octanol (b.p. 194–195 °C) obtained from Eastman Organic Chemicals was redistilled.

The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:

Solubility: Nothing specified.

Temperature: ±0.05 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

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Variables:	**Prepared by:**
$t/^\circ\mathrm{C}=25$	A. Goto and R. Goto

Solubility of propylparaben in 1-octanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\,cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.8809	26.6	0.200

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Octanol (Eastman-Kodak No. 50) was used.

Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[33] K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:	**Prepared by:**
$t/^\circ\mathrm{C}=25-40$	A. Goto and R. Goto

Solubility of propylparaben in 1-octanol

Temperature	Solubility	
$t/^\circ\mathrm{C}$	x_1	w_1[a] (compiler)
25	0.200	0.266
30	0.228	0.290
35	0.271	0.339
40	0.298	0.370

[a] In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde propylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

The purity of 1-octanol established by refractive-index and dielectric-constant measurements was 99 mol %.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[35] S.H. Yalkowsky, S.C. Valvani, and T.J. Roseman, J. Pharm. Sci. **72**, 866 (1983).

Variables:	**Prepared by:**
$t/^\circ\mathrm{C}=30$	A. Goto and R. Goto

Solubility of propylparaben in 1-octanol at 30 °C

Solubility	
$\log_{10} x_1$	x_1 (compiler)
−0.55	0.28

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 35 for the ethylparaben–1-octanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

Propylparaben of purest grade was obtained from commercial sources (Aldrich, Eastman, and Fluka) and was used as received.

Reagent-grade octanol was obtained from Aldrich.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36] A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).

Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of propylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\,dm^{-3}}=2.16$.

Auxiliary Information

Methods/Apparatus/Procedure:

A slight excess of the solute was introduced into 1-octanol, and after 2 days equilibration at 298.2 K, the solute concentrations were determined spectrophotometrically at 258 nm [A.E. Beezer, W.H. Hunter, and D. E. Storey, J. Pharm. Pharmacol. **35**, 350 (1983)].

Source and Purity of Materials:

The propylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%.

1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

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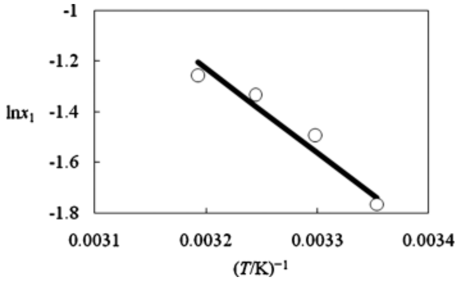

FIG. 29. Fitting curve of Eq. (2) and the observed data for propylparaben in 1-decanol.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 60. Summary of experimental solubility data of propylparaben in 1-decanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	21.7	17.1	Spectroscopy, Gravimetry	32
298.2	21.7	17.1	Spectroscopy	33
303.2	24.8	22.5	Spectroscopy	33
308.2	29.0	26.4	Spectroscopy	33
313.2	31.2	28.5	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/\text{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of propylparaben in 1-decanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 60). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 29, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.978

Sample size: 5 data points

p-value (F test): 0.004

Constants: $A=-3330\pm414$, $C=9.427\pm1.362$

White circles in Fig. 29 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-3330/T+9.427$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.978, as shown in Fig. 29. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 61 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 61. Observed data and recommended values calculated according to Eq. (2) for propylparaben in 1-decanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	17.1	17.6
303.2	22.5	21.1
308.2	26.4	25.3
313.2	28.5	30.0

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/°\text{C}=25$	A. Goto and R. Goto

Solubility of propylparaben in 1-decanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.8732	21.7	0.171

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

The source of 1-decanol was not reported.

Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°\text{C}=25-40$	A. Goto and R. Goto

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Solubility of propylparaben in 1-decanol

Temperature	Solubility	
$t/°\mathrm{C}$	x_1	w_1[a] (compiler)
25	0.171	0.217
30	0.225	0.248
35	0.264	0.290
40	0.285	0.312

[a] In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde propylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

The purity of 1-decanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

2.2.1.4. Butylparaben

Components:

(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]

(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan

Rensuke Goto, University of Shizuoka, Shizuoka, Japan

Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 62. Summary of experimental solubility data of butylparaben in methanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	75.5	33.6	Spectroscopy, Gravimetry	32
298.2	75.5	33.6	Spectroscopy	33
303.2	77.9	36.9	Spectroscopy	33
308.2	83.4	45.7	Spectroscopy	33
313.2	85.4	49.1	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of butylparaben in methanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 62). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 30, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

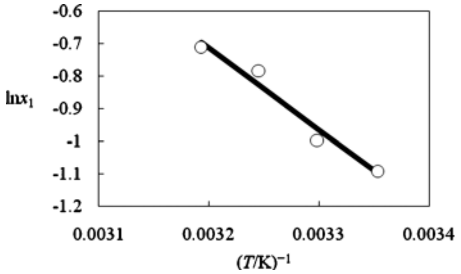

FIG. 30. Fitting curve of Eq. (2) and the observed data for butylparaben in methanol.

Multiple correlation coefficient: 0.986

Sample size: 5 data points

p-value (F test): 0.002

Constants: $A=-2493\pm246$, $C=7.264\pm0.808$

White circles in Fig. 30 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2493/T+7.264$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.986, as shown in Fig. 30. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 63 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 63. Observed data and recommended values calculated according to Eq. (2) for butylparaben in methanol

T/K	$100x_1(\mathrm{obs})$	$100x_1(\mathrm{rec})$
298.2	33.6	33.4
303.2	36.9	38.3
308.2	45.7	43.8
313.2	49.1	49.8

Components:

(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]

(2) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:

[32] A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:

$t/°\mathrm{C}=25$

Prepared by:

A. Goto and R. Goto

Solubility of butylparaben in methanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.9896	75.5	0.336

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Methanol (Fisher certified) was used.

Butylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°C=25-40$	A. Goto and R. Goto

Solubility of butylparaben in methanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.336	0.755
30	0.369	0.779
35	0.457	0.834
40	0.491	0.854

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde butylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

The source and the purity of methanol were not reported.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

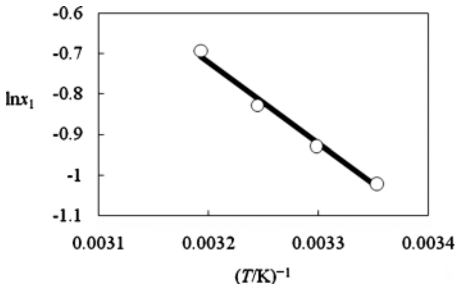

FIG. 31. Fitting curve of Eq. (2) and the observed data for butylparaben in ethanol.

Critical Evaluation

TABLE 64. Summary of experimental solubility data of butylparaben in ethanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	70.3	36.0	Spectroscopy, Gravimetry	32
298.2	70.3	36.0	Spectroscopy	33
303.2	73.4	39.5	Spectroscopy	33
308.2	76.6	43.7	Spectroscopy	33
313.2	80.7	50.0	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of butylparaben in ethanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 64). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 31, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.996

Sample size: 5 data points

p-value (F test): 0.000

Constants: $A=-1991\pm109$, $C=5.649\pm0.359$

White circles in Fig. 31 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1991/T+5.649$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.996, as shown in Fig. 31. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 65 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

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TABLE 65. Observed data and recommended values calculated according to Eq. (2) for butylparaben in ethanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	36.0	35.8
303.2	39.5	39.9
308.2	43.7	44.4
313.2	50.0	49.2

Components:
(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/^\circ C=25$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in ethanol at 25 °C

Density	Solubility[a]	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$ (compiler)	x_1
0.9730	70.3	0.360

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Absolute ethanol was obtained from U.S. Industrial Chemical Co. Butylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
$t/^\circ C=25-40$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in ethanol

Temperature	Solubility	
$t/^\circ C$	x_1	w_1[a] (compiler)
25	0.360	0.703
30	0.395	0.734
35	0.437	0.766
40	0.500	0.807

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde butylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value. Ethanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of 1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Propanol (propan-1-ol, propyl alcohol); $C_{11}H_{14}O_3$; [71-23-8]

Evaluators:
Ayako Goto, University of Shizuoka, Shizuoka, Japan
Rensuke Goto, University of Shizuoka, Shizuoka, Japan
Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 66. Summary of experimental solubility data of butylparaben in 1-propanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	64.7	36.1	Spectroscopy, Gravimetry	34
298.2	64.7	35.5	Spectroscopy, Gravimetry	32
298.2	64.7	35.5	Spectroscopy	33
303.2	68.2	40.2	Spectroscopy	33
308.2	72.9	45.8	Spectroscopy	33
313.2	76.3	50.2	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of butylparaben in 1-propanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 66). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 32, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

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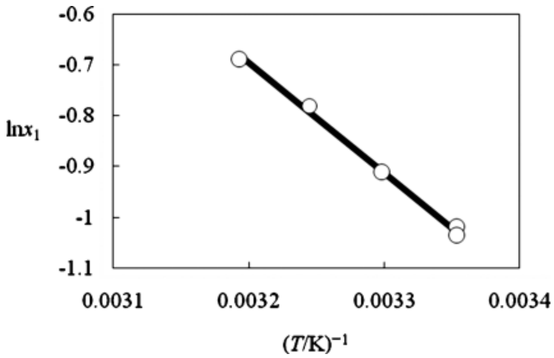

FIG. 32. Fitting curve of Eq. (2) and the observed data for butylparaben in 1-propanol.

Multiple correlation coefficient: 0.998
Sample size: 6 data points
p-value (F test): 0.000
Constants: $A=-2166\pm 67$, $C=6.243\pm 0.221$

White circles in Fig. 32 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2166/T+6.234$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.998, as shown in Fig. 32. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 67 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 67. Observed data and recommended values calculated according to Eq. (2) for butylparaben in 1-propanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	36.1	35.7
303.2	40.2	40.3
308.2	45.8	45.2
313.2	50.2	50.6

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=25$	A. Goto and R. Goto

Solubility of butylparaben in 1-propanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	w_1[a] (compiler)	x_1
0.9724	0.6466	0.361

[a]In the original paper, the solubility was given as grams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
Fisher certified grade 1-propanol (b.p. 96.9–97.2 °C) was used without further purification.
The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=25$	A. Goto and R. Goto

Solubility of butylparaben in 1-propanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.9719	64.7	0.355

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
1-Propanol (Baker analyzed) was used.
Butylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

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Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) 1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]	[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).
Variables:	**Prepared by:**
$t/°C=25-40$	A. Goto and R. Goto

Solubility of butylparaben in 1-propanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.355	0.647
30	0.402	0.682
35	0.458	0.729
40	0.502	0.763

[a]In the original paper, the solubility was given as mg/g of solution

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde butylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

1-Propanol (J.T. Baker) was of absolute reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:	**Evaluators:**
(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	Ayako Goto, University of Shizuoka, Shizuoka, Japan Rensuke Goto, University of Shizuoka, Shizuoka, Japan Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 68. Summary of experimental solubility data of butylparaben in 1-butanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	60.1	36.5	Spectroscopy, Gravimetry	34
298.2	60.1	36.4	Spectroscopy, Gravimetry	32
298.2	60.1	36.4	Spectroscopy	33
303.2	62.5	38.8	Spectroscopy	33
308.2	67.2	43.9	Spectroscopy	33
313.2	72.5	50.1	Spectroscopy	33

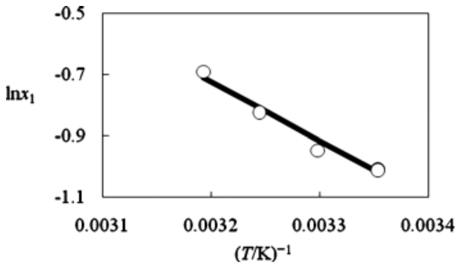

FIG. 33. Fitting curve of Eq. (2) and the observed data for butylparaben in 1-butanol.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/K=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of butylparaben in 1-butanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 68). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 33, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.989

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-1911\pm 146$, $C=5.392\pm 0.481$

White circles in Fig. 33 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1911/T+5.392$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.989, as shown in Fig. 33. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 69 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 69. Observed data and recommended values calculated according to Eq. (2) for butylparaben in 1-butanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	36.5	36.1
303.2	38.8	40.2
308.2	43.9	44.5
313.2	50.1	49.1

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]	[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

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Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-butanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	w_1[a] (compiler)	x_1
0.9592	0.6005	0.365

[a] In the original paper, the solubility was given as grams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
Fisher certified grade 1-butanol (b.p. 116.6–117.8 °C) was used without further purification.

The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:
[32] A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-butanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.9612	60.1	0.364

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
The source of 1-butanol was not reported.

Butylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Original Measurements:
[33] K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
$t/°C=25–40$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-butanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.364	0.601
30	0.388	0.625
35	0.439	0.672
40	0.501	0.725

[a] In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde butylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

1-Butanol (Mallinckrodt) was of analytical reagent quality. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Evaluators:
Ayako Goto, University of Shizuoka, Shizuoka, Japan
Rensuke Goto, University of Shizuoka, Shizuoka, Japan
Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 70. Summary of experimental solubility data of butylparaben in 1-hexanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	52.9	37.1	Spectroscopy, Gravimetry	34
298.2	52.6	36.9	Spectroscopy, Gravimetry	32
298.2	52.6	36.9	Spectroscopy	33
303.2	55.2	39.5	Spectroscopy	33
308.2	60.3	44.4	Spectroscopy	33
313.2	66.1	50.7	Spectroscopy	33

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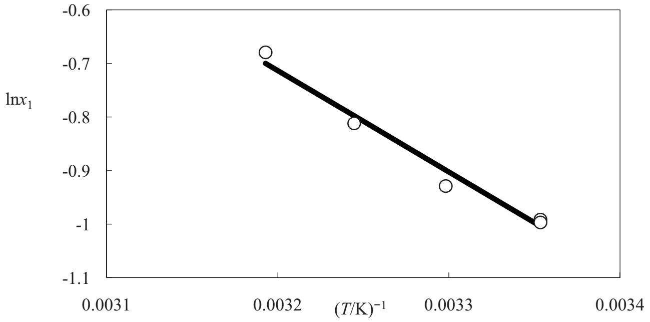

FIG. 34. Fitting curve of Eq. (2) and the observed data for butylparaben in 1-hexanol.

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 3

The range of temperature: $T/\mathrm{K}=298.2-313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of butylparaben in 1-hexanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 70). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 34, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.990

Sample size: 6 data points

p-value (F test): 0.000

Constants: $A=-1892\pm 137$, $C=5.341\pm 0.454$

White circles in Fig. 34 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-1892/T+5.341$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.990, as shown in Fig. 34. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 71 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 71. Observed data and recommended values calculated according to Eq. (2) for butylparaben in 1-hexanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	37.1	36.7
303.2	39.5	40.7
308.2	44.4	45.0
313.2	50.7	49.7

Components:

(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]

(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:

[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

Variables:

$t/{}^\circ\mathrm{C}=25$

Prepared by:

A. Goto and R. Goto

Solubility of butylparaben in 1-hexanol at 25 °C

Density	Solubility[a]	
$\rho/\mathrm{g\ cm^{-3}}$	w_1[a] (compiler)	x_1 (compiler)
0.9467	0.5292	0.371

[a]In the original paper, the solubility was given as grams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

1-Hexanol (b.p. 156.5–157.5 °C) obtained from Eastman Organic Chemicals was redistilled.

The butylparaben (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:

Solubility: Nothing specified.

Temperature: ±0.05 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]

(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:

[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:

$t/{}^\circ\mathrm{C}=25$

Prepared by:

A. Goto and R. Goto

Solubility of butylparaben in 1-hexanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	w_1[a] (compiler)	x_1 (compiler)
0.9413	52.6	0.369

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Hexanol (Eastman-Kodak No. 50) was used.

Butylparaben was obtained from Matheson, Coleman and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]

(2) 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3]

Original Measurements:

[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:

$t/°C=25–40$

Prepared by:

A. Goto and R. Goto

Solubility of butylparaben in 1-hexanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.369	0.526
30	0.395	0.552
35	0.444	0.603
40	0.507	0.661

[a] In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde butylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

The purity of 1-hexanol established by refractive-index and dielectric-constant measurements was 99 mol %.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, butyl ester (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]

(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Evaluators:

Ayako Goto, University of Shizuoka, Shizuoka, Japan

Rensuke Goto, University of Shizuoka, Shizuoka, Japan

Hiroshi Fukuda, Kitasato University, Tokyo, Japan

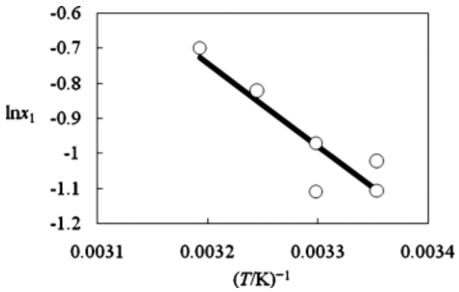

FIG. 35. Fitting curve of Eq. (2) and the observed data for butylparaben in 1-octanol.

Critical Evaluation

TABLE 72. Summary of experimental solubility data of butylparaben in 1-octanol

T/K	$c_1/mol\ dm^{-3}$	$100w_1$	$100x_1$	Analytical method	Reference
298.2		45.7	36.0	Spectroscopy, Gravimetry	34
298.2		45.7	33.1	Spectroscopy, Gravimetry	32
298.2		45.7	33.1	Spectroscopy	33
298.2	2.39			Spectroscopy	36
303.2		47.6	37.9	Spectroscopy	33
303.2			33.0	Spectroscopy	35
308.2		53.9	44.0	Spectroscopy	33
313.2		59.5	49.7	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 5

The range of temperature: $T/K=298.2–313.2$

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of butylparaben in 1-octanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 72). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 35, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.910

Sample size: 7 data points

p-value (F test): 0.004

Constants: $A=-2349\pm478$, $C=6.774\pm1.577$

White circles in Fig. 35 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-2349/T+6.774$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.910, as shown in Fig. 35. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

Table 73 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

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TABLE 73. Observed data and recommended values calculated according to Eq. (2) for butylparaben in 1-octanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	36.0	33.2
303.2	37.9	37.8
308.2	44.0	42.8
313.2	49.7	48.4

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

Variables:
t/ °C=25

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-octanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	w_1[a]	x_1
0.9291	0.4565	0.360

[a]In the original paper, the solubility was given as grams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
1-Octanol (b.p. 194–195 °C) obtained from Eastman Organic Chemicals was redistilled.

The butylparaben (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
t/ °C=25

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-octanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.9346	45.7	0.331

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
1-Octanol (Eastman-Kodak No. 50) was used.
Butylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (n-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
t/ °C=25–40

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-octanol

Temperature	Solubility	
t/ °C	x_1	w_1[a] (compiler)
25	0.331	0.457
30	0.379	0.476
35	0.440	0.539
40	0.497	0.595

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde butylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.

The purity of 1-octanol established by refractive-index and dielectric-constant measurements was 99 mol %.

Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of ±0.1 °C.

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Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[35]S.H. Yalkowsky, S.C. Valvani, and T.J. Roseman, J. Pharm. Sci. **72**, 866 (1983).

Variables:
$t/°C=30$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-octanol at 30 °C

Solubility	
$\log_{10} x_1$	x_1 (compiler)
−0.48	0.33

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 35 for the ethylparaben–1-octanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
Reagent-grade octanol was obtained from Aldrich.

Butylparaben of purest grade was obtained from commercial sources (Aldrich, Eastman, and Fluka) and was used as received.

Estimated Errors:
Nothing specified.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:
[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).

Variables:
$T/K=298.2$

Prepared by:
A. Goto and R. Goto

The solubility of butylparaben in 1-octanol at 298.2 K was reported as $c_1/\text{mol dm}^{-3}=2.39$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental detail is given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:
The butylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%.

1-Octanol was of Anala R grade.

Estimated Errors:
Nothing specified.

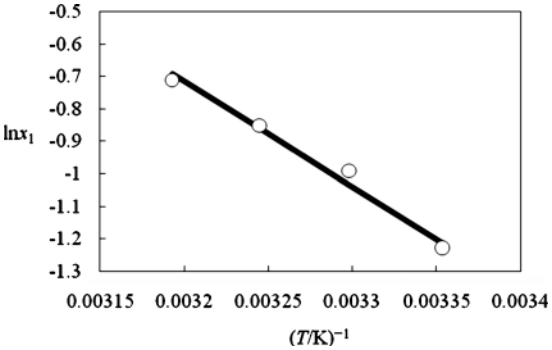

FIG. 36. Fitting curve of Eq. (2) and the observed data for butylparaben in 1-decanol.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]

Evaluators:
Ayako Goto, University of Shizuoka, Shizuoka, Japan
Rensuke Goto, University of Shizuoka, Shizuoka, Japan
Hiroshi Fukuda, Kitasato University, Tokyo, Japan

Critical Evaluation

TABLE 74. Summary of experimental solubility data of butylparaben in 1-decanol

T/K	$100w_1$	$100x_1$	Analytical method	Reference
298.2	39.2	29.3	Spectroscopy, Gravimetry	32
298.2	39.2	29.3	Spectroscopy	33
303.2	42.1	37.1	Spectroscopy	33
308.2	47.7	42.7	Spectroscopy	33
313.2	54.2	49.1	Spectroscopy	33

The critical evaluation was carried out as described in Sec. 2.1.1.1 for salicylic acid in *n*-heptane.

The number of publications: 2

The range of temperature: $T/K=298.2-313.2$.

The units: mass percent and mole fraction

Analytical methods: spectroscopy and gravimetry

Data for the solubility of butylparaben in 1-decanol expressed by mole fraction were fitted to Eqs. (1) and (2) given in Sec. 1.3 (Table 74). The data points nearly agree with Eq. (2) over the whole range of temperatures, as shown in Fig. 36, but they deviated from Eq. (1). Multiple regression analysis according to Eq. (2) yielded the following results:

Multiple correlation coefficient: 0.994

Sample size: 5 data points

p-value (F test): 0.001

Constants: $A=-3246\pm 212$, $C=9.672\pm 0.698$

White circles in Fig. 36 represent the observed data and the black line corresponds to calculated values according to Eq. (2) ($\ln x_1=-3246/T+9.672$). The observed data fit closely with the calculated values in the range of 298.2–313.2 K, with the multiple correlation coefficient of 0.994, as shown in Fig. 36. Therefore, the calculated value at each measured temperature is reasonably considered as a recommended value over the whole range of temperature.

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Table 75 shows the observed data in the range of 298.2–313.2 K and the recommended values calculated from Eq. (2) at each temperature.

TABLE 75. Observed data and recommended values calculated according to Eq. (2) for butylparaben in 1-decanol

T/K	$100x_1$(obs)	$100x_1$(rec)
298.2	29.3	29.7
303.2	37.1	35.6
308.2	42.7	42.3
313.2	49.1	50.1

Components:
(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
t/°C=25

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-decanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a]	x_1
0.9313	39.2	0.293

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
The source of 1-decanol was not reported.
Butylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (n-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Decanol (decan-1-ol, decyl alcohol); $C_{10}H_{22}O$; [112-30-1]

Original Measurements:
[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:
t/°C=25–40

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-decanol

Temperature	Solubility[a]	
t/°C	x_1	w_1 (compiler)
25	0.293	0.392
30	0.371	0.421
35	0.427	0.477
40	0.491	0.542

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
Spectrograde butylparaben was purchased from Matheson Coleman and Bell Co. The melting point was within 1 °C of the literature value.
The purity of 1-decanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:
Solubility: Precision within 2.5%.
Temperature: Precision of ±0.1 °C.

2.2.2. Data for paraben–organic compound systems

2.2.2.1. Methylparaben

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) Hydrocarbons (alkanes):
n-Pentane (pentane); C_5H_{12}; [109-66-0]
n-Hexane (hexane); C_6H_{14}; [110-54-3]
n-Heptane (heptane); C_7H_{16}; [142-82-5]
n-Nonane (nonane); C_9H_{20}; [111-84-2]
n-Decane (decane); $C_{10}H_{22}$; [124-18-5]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
t/°C=25

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in hydrocarbons at 25 °C

	Molar volume of solvent	Solubility
Solvent	v_2/cm^3 mol^{-1}	10^4x_1
n-Pentane	116.1	0.63
n-Hexane	131.6	0.77
n-Heptane	147.5	0.83
n-Nonane	179.7	1.06
n-Decane	195.9	1.21

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The detail is given in the compilation of Ref. 19 for the methylparaben–ethanol system in Sec. 2.2.1.1.

Estimated Errors:

Solubility: Errors were below 3%.

Temperature: Precision of ±0.2 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=288.2$, 293.2, and 298.2	A. Goto and R. Goto

Solubility of methylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^3c_1/\mathrm{mol\ dm^{-3}}$
288.2	1.09
293.2	2.50
298.2	2.21

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental detail is given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The methylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. *n*-Hexane was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=25$	A. Goto and R. Goto

Solubility of methylparaben in 1-pentanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.8819	24.6	0.149

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Pentanol (Eastman-Kodak No. 50) was used.

Methylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/{}^\circ\mathrm{C}=25$	A. Goto and R. Goto

Solubility of methylparaben in 1-pentanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
108.6	0.1528

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The detail is given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: Errors were below 3%.

Temperature: Precision of ±0.2 °C.

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Components:

(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]

(2) 1-Heptanol (heptan-1-ol, heptyl alcohol); $C_7H_{16}O$; [111-70-6]

Original Measurements:

[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:

$t/°C=25$

Prepared by:

A. Goto and R. Goto

Solubility of methylparaben in 1-heptanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
141.9	0.1483

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]

(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:

[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:

$t/°C=25$

Prepared by:

A. Goto and R. Goto

Solubility of methylparaben in 1-octanol at 25 °C

Density	Solubility	
$\rho/\mathrm{g\ cm^{-3}}$	$100w_1$[a] (compiler)	x_1
0.8712	14.7	0.111

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Octanol (Eastman-Kodak No. 50) was used.

Methylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]

(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]

Original Measurements:

[33]K.S. Alexander, J.W. Mauger, H. Petersen, Jr., and A.N. Paruta, J. Pharm. Sci. **66**, 42 (1977).

Variables:

$t/°C=25-40$

Prepared by:

A. Goto and R. Goto

Solubility of methylparaben in 1-octanol

Temperature	Solubility	
$t/°C$	x_1	w_1[a] (compiler)
25	0.111	0.147
30	0.151	0.172
35	0.166	0.188
40	0.172	0.195

[a]In the original paper, the solubility was given as mg/g of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 33 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

Spectrograde methylparaben was purchased from Matheson Coleman and Bell Co. Melting point was within 1 °C of literature values.

1-Octanol was 99 mol %. The purity of the alcohol was established by refractive-index and dielectric-constant measurements.

Estimated Errors:

Solubility: Precision within 2.5%.

Temperature: Precision of ±0.1 °C.

Components:

(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]

(2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_8O_3$; [111-87-5]

Original Measurements:

[35]S.H. Yalkowsky, S.C. Valvani, and T.J. Roseman, J. Pharm. Sci. **72**, 866 (1983).

Variables:

$t/°C=30$

Prepared by:

A. Goto and R. Goto

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Solubility of methylparaben in 1-octanol at 30 °C

Solubility	
$\log_{10} x_1$	x_1 (compiler)
−0.96	0.11

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 35 for the ethylparaben–1-octanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

Methylparaben of purest grade was obtained from commercial sources (Aldrich, Eastman, and Fluka) and was used as received.

1-Octanol was of reagent grade.

Estimated Errors:

Nothing specified.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of methylparaben in 1-octanol at 25 °C

Molar volume of solvent	Solubility
$v_2/\mathrm{cm}^3\,\mathrm{mol}^{-1}$	x_1
158.4	0.1381

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/K=298.2$	A. Goto and R. Goto

The solubility of methylparaben in 1-octanol at 298.2 K was reported as $c_1/\mathrm{mol\,dm^{-3}}=0.71$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The methylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%.

1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_{18}O$; [99-76-3] (2) Diols and triols: 1,2-Ethandiol (ethane-1,2-diol, ethylene glycol); $C_2H_6O_2$; [107-21-1] 1,2-Propandiol (propane-1,2-diol, propylene glycol); $C_3H_8O_2$; [57-55-6] 1,3-Propanediol (propane-1,3-diol, trimethylene glycol); $C_3H_8O_2$; [504-63-2] 1,4-Butanediol (butane-1,4-diol, tetramethylene glycol); $C_4H_{10}O_2$; [110-63-4] 1,2,3-Propanetriol (propane-1,2,3-triol, glycerol); $C_3H_8O_3$; [56-81-5]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

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Solubility of methylparaben in diols and triols at 25 °C

	Molar volume of solvent	Solubility
Solvent	$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
Ethylene glycol	55.9	0.0480
Propylene glycol	73.7	0.0941
Trimethylene glycol	72.5	0.0766
1,4-Butanediol	88.6	0.1202
Glycerol	73.2	0.0064

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The detail is given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Solubility: The experimental variation was below 3%.
Temperature: Precision of ±0.2 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) Ethers:
Ethane, 1,1′-oxybis- (ethoxyethane, diethyl ether); $C_4H_{10}O$; [60-29-7]
Propane, 1,1′-oxybis- (1-propoxypropane, dipropyl ether); $C_6H_{14}O$; [111-43-3]
Butane, 1,1′-oxybis- (2-butoxyethanol, dibutyl ether); $C_8H_{18}O$; [142-96-1]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°\mathrm{C}=25$.

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in ethers at 25 °C

	Molar volume of solvent	Solubility
Solvent	$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
Diethyl ether	104.8	0.0840
Dipropyl ether	139.4	0.0314
Dibutyl ether	170.4	0.0268

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The detail is given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Solubility: The experimental variation was below 3%.
Temperature: Precision of ±0.2 °C

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) Carboxylic acids:
Acetic acid; $C_2H_4O_2$; [64-19-7]
Propionic acid (propanoic acid); $C_3H_6O_2$; [79-09-4]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°\mathrm{C}=25$

Prepared by:
A. Goto and R. Goto

Solubility of methylparaben in carboxylic acids at 25 °C

	Molar volume of solvent	Solubility
Solvent	$v_2/\mathrm{cm^3\ mol^{-1}}$	x_1
Acetic acid	57.6	0.0532
Propionic acid	75.0	0.0386

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The detail is given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Solubility: Errors were below 3%.
Temperature: Precision of ±0.2 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3]
(2) Acetates:
Acetic acid, ethyl ester (ethyl acetate); C_4H_8O; [141-78-6]
Acetic acid, propyl ester (propyl acetate); $C_5H_{10}O_2$; [109-60-4]
Acetic acid, butyl ester (butyl acetate); $C_6H_{12}O_2$; [123-86-4]
Acetic acid, hexyl ester (hexyl acetate); $C_8H_{16}O_2$; [142-92-7]

Original Measurements:
[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:
$t/°\mathrm{C}=25$

Prepared by:
A. Goto and R. Goto

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Solubility of methylparaben in acetates at 25 °C

Solvent	Molar volume of solvent v_2/cm^3 mol^{-1}	Solubility x_1
Ethyl acetate	98.5	0.1270
Propyl acetate	115.7	0.1366
Butyl acetate	132.6	0.1326
Hexyl acetate	164.5	0.1164

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The detail is given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) Methane, 1,1′-sulfinylbis-(methylsulfinylmethane, dimethyl sulfoxide); C_2H_6OS; [67-68-5]	[19] A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:	Prepared by:
t/°C=25	A. Goto and R. Goto

The solubility of methylparaben in dimethyl sulfoxide at 25 °C was reported as x_1=0.5839.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The detail is given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) Amides: Formamide; CH_3NO; [75-12-7] Formamide, *N*-methyl- (*N*-methylformamide, methylformamide); C_2H_5NO; [123-39-7] Formamide, *N*,*N*-dimethyl- (*N*,*N*-dimethylformamide, dimethylformamide); C_3H_7NO; [68-12-2] Formamide, *N*,*N*-diethyl- (*N*,*N*-diethylformamide, diethylformamide); $C_5H_{11}NO$; [617-84-5] Acetamide, *N*,*N*-dimethyl- (*N*,*N*-dimethylacetamide, dimethylacetamide); C_4H_9NO; [127-19-5] Acetamide, *N*,*N*-diethyl- (*N*,*N*-diethylacetamide, diethylacetamide); $C_6H_{13}NO$; [685-91-6]	[19] A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).

Variables:	Prepared by:
t/°C=25	A. Goto and R. Goto

Solubility of methylparaben in amides at 25 °C

Solvent	Molar volume of solvent v_2/cm^3 mol^{-1}	Solubility x_1
Formamide	39.9	0.0765
N-Methylformamide	59.1	0.2981
N,*N*-Dimethylformamide	77.4	0.4605
N,*N*-Diethylformamide	112.0	0.4907
N,*N*-Dimethylacetamide	93.0	0.5418
N,*N*-Diethylacetamide	126.6	0.5299

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:

The detail is given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:

Solubility: The experimental variation was below 3%.

Temperature: Precision of ±0.2 °C.

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Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) Pyridine; C_5H_5N; [110-86-1]	[19]A. Martin, P.L. Wu, and A. Beerbower, J. Pharm. Sci. **73**, 188 (1984).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

The solubility of methylparaben in pyridine at 25 °C was reported as $x_1=0.3243$.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Source and Purity of Materials:
The details are given in the compilation of Ref. 19 for the 4-hydroxybenzoic acid–ethanol system in Sec. 2.1.2.3.

Estimated Errors:
Solubility: The experimental variation was below 3%.
Temperature: Precision of ±0.2 °C.

2.2.2.2. Ethyl-, propyl-, and butylparaben

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991)
Variables:	**Prepared by:**
$T/K=288.2$, 293.2, and 298.2	A. Goto and R. Goto

Solubility of ethylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^4c_1/\mathrm{mol\ dm^{-3}}$
288.2	2.56
293.2	4.38
298.2	5.33

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:
The ethylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. *n*-Hexane was of Anala R grade.

Estimated Errors:
Nothing specified.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/K=288.2$, 293.2, and 298.2	A. Goto and R. Goto

Solubility of propylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^3c_1/\mathrm{mol\ dm^{-3}}$
288.2	0.667
293.2	0.867
298.2	1.28

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:
The propylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. *n*-Hexane was of Anala R grade.

Estimated Errors:
Nothing specified.

Components:	Original Measurements:
(1) Benzoic acid, 4-hydroxy-, butyl ester; (*n*-butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/K=288.2$, 293.2, and 298.2	A. Goto and R. Goto

Solubility of butylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^3c_1/\mathrm{mol\ dm^{-3}}$
288.2	1.39
293.2	2.23
298.2	2.54

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The butylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%.

n-Hexane was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]	[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of ethylparaben in 1-pentanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	w_1[a]	x_1
0.8961	0.2987	0.184

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

The source and the purity of 1-pentanol were not reported.

The ester (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:

Solubility: Nothing specified.

Temperature: ±0.05 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, ethyl ester (ethyl 4-hydroxybenzoate, ethylparaben); $C_9H_{10}O_3$; [120-47-8] (2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]	[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of ethylparaben in 1-pentanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a] (compiler)	x_1
0.8911	29.9	0.185

[a]In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:

1-Pentanol (Eastman-Kodak No. 50) was used.

Ethylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]	[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).
Variables:	**Prepared by:**
$t/°C=25$	A. Goto and R. Goto

Solubility of propylparaben in 1-pentanol at 25 °C

Density	Solubility[a]	
ρ/g cm^{-3}	w_1[a]	x_1
0.9059	0.3623	0.217

[a]In the original paper, the solubility was given as grams of the ester per gram of saturated solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:

The source and the purity of 1-pentanol were not reported.

The propylparaben (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:

Solubility: Nothing specified.

Temperature: ±0.05 °C.

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Components:
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl 4-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3]
(2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of propylparaben in 1-pentanol at 25 °C

Density	Solubility[a]	
ρ/g cm^{-3}	$100w_1$ (compiler)	x_1
0.8994	36.2	0.212

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
1-Pentanol (Eastman-Kodak No. 50) was used.
Propylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]

Original Measurements:
[34]F.A. Restaino and A.N. Martin, J. Pharm. Sci. **53**, 636 (1964).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-pentanol at 25 °C

Density	Solubility[a]	
ρ/g cm^{-3}	w_1[a]	x_1
0.9527	0.5579	0.364

[a] In the original paper, the solubility was given as grams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 34 for the ethylparaben–1-propanol system in Sec. 2.2.1.2.

Source and Purity of Materials:
The source and the purity of 1-pentanol were not reported.
The butylparaben (purified grade) was recrystallized from chloroform until a sharp melting point was obtained.

Estimated Errors:
Solubility: Nothing specified.
Temperature: ±0.05 °C.

Components:
(1) Benzoic acid, 4-hydroxy-, 1-butyl ester (butyl 4-hydroxybenzoate, butylparaben); $C_{11}H_{14}O_3$; [94-26-8]
(2) 1-Pentanol (pentan-1-ol, pentyl alcohol); $C_5H_{12}O$; [71-41-0]

Original Measurements:
[32]A.N. Paruta, J. Pharm. Sci. **58**, 216 (1969).

Variables:
$t/°C=25$

Prepared by:
A. Goto and R. Goto

Solubility of butylparaben in 1-pentanol at 25 °C

Density	Solubility	
ρ/g cm^{-3}	$100w_1$[a]	x_1
0.9547	55.8	0.363

[a] In the original paper, the solubility was given as milligrams of the ester per gram of solution.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 32 for the methylparaben–methanol system in Sec. 2.2.1.1.

Source and Purity of Materials:
1-Pentanol (Eastman-Kodak No. 50) was used.
Butylparaben was obtained from Matheson, Coleman, and Bell.

Estimated Errors:
Solubility: Nothing specified.
Temperature: Precision of ±0.1 °C.

2.2.2.3. Hexyl-, heptyl-, octyl-, and decylparaben

Components:
(1) Benzoic acid, 4-hydroxy-, hexyl ester (hexyl *p*-hydroxybenzoate, hexylparaben); $C_{13}H_{18}O_3$; [1083-27-8]
(2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]

Original Measurements:
[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).

Variables:
$T/K=288.2$, 293.2, and 298.2

Prepared by:
A. Goto and R. Goto

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Solubility of hexylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^2c_1/\mathrm{mol\ dm^{-3}}$
288.2	1.90
293.2	3.00
298.2	3.90

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The hexylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. *n*-Hexane was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, heptyl ester (heptyl *p*-hydroxybenzoate, heptylparaben); $C_{14}H_{20}O_3$; [1085-12-7] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=288.2$, 293.2, and 298.2	A. Goto and R. Goto

Solubility of heptylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^2c_1/\mathrm{mol\ dm^{-3}}$
288.2	1.0
293.2	2.80
298.2	3.20

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The heptylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. *n*-Hexane was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, octyl ester (octyl *p*-hydroxybenzoate, octylparaben); $C_{15}H_{22}O_3$; [1219-38-1] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=288.2$, 293.2, and 298.2	A. Goto and R. Goto

Solubility of octylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^2c_1/\mathrm{mol\ dm^{-3}}$
288.2	0.678
293.2	1.10
298.2	1.80

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The octylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. *n*-Hexane was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, decyl ester (decyl *p*-hydroxybenzoate, decylparaben); $C_{17}H_{26}O_3$; [99-76-3] (2) *n*-Hexane (hexane); C_6H_{14}; [110-54-3]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=288.2$, 293.2, and 298.2	A. Goto and R. Goto

Solubility of decylparaben in *n*-hexane

Temperature	Solubility
T/K	$10^3c_1/\mathrm{mol\ dm^{-3}}$
288.2	3.08
293.2	4.57
298.2	7.16

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

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Source and Purity of Materials:

The decylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity specified as >99.5%. *n*-Hexane was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, hexyl ester (hexyl *p*-hydroxybenzoate, hexylparaben); $C_{13}H_{18}O_3$; [1083-27-8] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of hexylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\ dm^{-3}}=6.39$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The hexylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. 1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, heptyl ester (heptyl 4-hydroxybenzoate, heptylparaben); $C_{14}H_{20}O_3$; [1085-12-7] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of heptylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\ dm^{-3}}=4.52$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The heptylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. 1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, octyl ester (octyl *p*-hydroxybenzoate, octylparaben); $C_{15}H_{22}O_3$; [1219-38-1] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of octylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\ dm^{-3}}=3.67$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The octylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. 1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, decyl ester (decyl *p*-hydroxybenzoate, decylparaben); $C_{17}H_{26}O_3$; [2664-60-0] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of decylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\ dm^{-3}}=1.96$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The decylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%. 1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

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2.2.2.4. Methylpropyl-, pentyl-, and benzylparaben

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, 2-methylpropyl ester (isobutyl *p*-hydroxybenzoate, isobutylparaben); $C_{11}H_{14}O_3$; [4247-02-3] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of isobutylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\ dm^{-3}}=2.81$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The isobutylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%.

1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, pentyl ester (pentyl *p*-hydroxybenzoate, pentylparaben); $C_{12}H_{16}O_3$; [6521-29-5] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of pentylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\ dm^{-3}}=3.96$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The pentylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity was specified as >99.5%.

1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, phenylmethyl ester (benzyl *p*-hydroxybenzoate, benzylparaben); $C_{14}H_{12}O_3$; [94-18-8] (2) 1-Octanol (octan-1-ol, octyl alcohol); $C_8H_{18}O$; [111-87-5]	[36]A.E. Beezer, S. Forster, W.-B. Park, and G.J. Rimmer, Thermochim. Acta **178**, 59 (1991).
Variables:	**Prepared by:**
$T/\mathrm{K}=298$	A. Goto and R. Goto

The solubility of benzylparaben in 1-octanol at 298 K was reported as $c_1/\mathrm{mol\ dm^{-3}}=9.76$.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 36 for the propylparaben–1-octanol system in Sec. 2.2.1.3.

Source and Purity of Materials:

The benzylparaben was the gift of Apin Chemicals Ltd. (Abingdon, Great Britain) and was used as received. The purity specified as >99.5%.

1-Octanol was of Anala R grade.

Estimated Errors:

Nothing specified.

2.3. Hydroxybenzoic acid salt–organic compound systems

2.3.1. 2-Hydroxybenzoic acid salt (Na)

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy-, monosodium salt (sodium salicylate); $C_7H_5NaO_3$; [54-21-7] (2) Methyl alcohol (methanol); CH_4O; [67-56-1]	[37]H. Henstock, J. Chem. Soc. **1934**, 1340.
Variables:	**Prepared by:**
$t/°\mathrm{C}=15$ and 67.2 (boiling point of solution)	H. Miyamoto and A. Goto

Solubility of sodium salicylate in methanol

Temperature	Solubility		
$t/°\mathrm{C}$	Original data[a]	w_1[b] (compiler)	$m_1/\mathrm{mol\ kg^{-1}}$ (compiler)
15	26.28	0.2081	1.641
67.2 (boiling point)	34.73	0.2578	2.169

[a] In the original paper, the solubility was given as grams of salt per 100 g of solvent.

[b] $w_1=m_1/\Sigma m_i$, where w_1 is the mass fraction of sodium salicylate. m_1 and Σm_i are mass of sodium salicylate and mass of solution, respectively.

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Auxiliary Information

Methods/Apparatus/Procedure:

The apparatus used for the measurements at 15 °C was similar to that described in [J.N. Bronsted and A. Petersen, J. Am. Chem. Soc. **43**, 2265 (1921)]. It was immersed in a thermostat. At boiling temperature, the solutions were made in a wide flask under reflux. To determine the quantities of solutes, portions of the saturated solutions were weighed at 15 °C in a graduated pipette of the type used by [F.D. Chattaway and W.J. Lambert, J. Chem. Soc. **107**, 1766 (1915)]; a filter thimble was introduced into the solution to separated undissolved salt. The contents being discharged into a weighing bottle, the pipette was washed with the boiling solvent, and the residue was weighed after evaporation of solvent; thus the weights of solute and solvent were both obtained.

Source and Purity of Materials:

Sodium salicylate was recrystallized twice from boiling methanol.

Methanol was purified by first removing acetone by Minuses' method, aldehyde was abstracted by treatment with iodine, and distillation with concentrated sulfuric acid removed basic substance as well as most of the water. Acid substances were removed by distillation from caustic potash, and the alcohol was distilled over metallic sodium; b.p. 66 °C at 758 mmHg.

Estimated Errors:

Solubility: Precision of ±1%.

Temperature: Precision of ±0.1 °C.

2.3.2. 2-Hydroxybenzoic acid salt (Ag)

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy-, silver salt (silver salicylate); $C_7H_5O_3Ag$; [35959-19-4] (2) Alcohols: Methyl alcohol (methanol); CH_4O; [67-56-1] Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	[38]I.M. Kolthoff, J.J. Lingane, and W.D. Larson, J. Am. Chem. Soc. **60**, 2512 (1938).

Variables:	**Prepared by:**
$t/°C=25$	H. Miyamoto

Solubility of silver salicylate in alcohols at 25 °C

Solvent	Solubility $10^4c_1/\text{mol dm}^{-3}$
Methanol	5.69
Ethanol	3.10

Auxiliary Information

Methods/Apparatus/Procedure:

Saturated solution of the silver salt was prepared in conductance cells through which a stream of previously dried nitrogen, saturated with the vapor of the solvent, was led to provide stirring. When the conductance had become constant, samples of the saturated aqueous solutions were withdrawn and analyzed for silver by the potentiometric method. The solubilities in ethanol and methanol were determined by the conductance method. The conductance cells were of the type used by [I.M. Kolthoff and A. Willman, J. Am. Chem. Soc. **56**, 1008 (1934)]. Their cell constants were determined in the usual way. The conductance of methanol at 25 °C varied from 2.9 to 5.0 and the range in the corresponding values for ethanol was from 0.4 to 1.2×10^{-4} S cm^{-1}. The conductance of the pure alcohol was subtracted from the observed conductivities where necessary.

Source and Purity of Materials:

Ethanol and methanol were refluxed over silver oxide, distilled and dehydrated with magnesium. The water content of methanol ranged from 0% to 0.03%, while that of ethanol varied from 0.01% to 0.07%.

The silver salt of the acid was precipitated from solutions of the corresponding sodium salt with a slight excess of silver nitrate. The precipitates were washed and recrystallized from hot water. The product was washed with water, then with ethanol, and air dried.

Estimated Errors:

Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 2-hydroxy-, silver salt (silver salicylate); $C_7H_5O_3Ag$ (Merck), $2(OH)C_6H_4CO_2Ag$ (Aldrich), $C_7H_6O_3Ag$ (CA); [35959-19-4] (2) Alcohols: Methyl alcohol (methanol); CH_4O; [67-56-1] Ethyl alcohol (ethanol); C_2H_6O; [64-17-5] 1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3] 1-Butanol, 3-methyl- (3-methylbutan-1-ol, isoamyl alcohol); $C_5H_{12}O$; [123-51-3] 1-Hexanol (hexan-1-ol, hexyl alcohol); $C_6H_{14}O$; [111-27-3] 1-Heptanol (*n*-heptan-1-ol, heptyl alcohol); $C_7H_{16}O$; [111-70-6]	[39]N.A. Izmailov and V.S. Chernyi, Zh. Fiz. Khim. **34**, 319 (1960) [Russ. J. Phys. Chem. (Engl. Transl.) **34**, 149 (1960)].

Variables:	**Prepared by:**
$t/°C=25$	H. Miyamoto

Solubility of silver salicylate in alcohols at 25 °C

Solvent	Solubility $10^4m_1/\text{mol kg}^{-1}$
Methanol	6.54
Ethanol	5.15
1-Butanol	1.11
Isoamyl alcohol	1.09
n-Hexyl alcohol	1.91
n-Heptyl alcohol	1.64

Auxiliary Information

Methods/Apparatus/Procedure:

The solubility determination of the silver salt used the radioactive isotope ^{110}Ag. The silver salt with solvent was placed in a tube, sealed and placed in an air thermostat. Equilibrium was reached in 16–18 h. The solution removed from the tube was centrifuged. The samples were withdrawn by a micropipette and run on to a disk of filter paper, dried, and sealed in tracing cloth or Cellophane. The prepared specimens were found on a cylindrical counter and their radioactivity was measured. The methods of preparing saturated solutions, sampling, and the radioactive measurement are described in [N.A. Izmailov and V.S. Chernyi, Zh. Fiz. Khim. **34**, 127 (1960); Russ. J. Phys. Chem. (Engl. Transl.) **34**, 59 (1960)]. The concentration of silver salicylate was analyzed for silver content.

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Source and Purity of Materials:
The silver salt of salicylic acid was prepared from silver nitrate labeled with radioactive ^{110}Ag and the sodium or potassium salts of the acid.
The solvents were carefully purified.
Estimated Errors:
Solubility: Relative accuracy was 1%–3% at a confidence limit of 0.95.
Temperature: Precision of ±0.5 °C.

Components: (1) Benzoic acid, 2-hydroxy-, silver salt (silver salicylate); C_7H_5OAg (Merck), $2(OH)C_6H_4CO_2Ag$ (Aldrich), $C_7H_6O_3Ag$ (CA); [35959-19-4] (2) Ketones: 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1] 2-Butanone (butan-2-one, methyl ethyl ketone); C_4H_8O; [78-93-3] 4-Heptanone (heptan-4-one, dipropyl ketone); $C_7H_{14}O$; [123-19-3]	**Original Measurements:** [39]N.A. Izmailov and V.S. Chernyi, Zh. Fiz. Khim. **34**, 319 (1960) [Russ. J. Phys. Chem. (Engl. Transl.) **34**, 149 (1960)].
Variables: $t/°C=25$	**Prepared by:** H. Miyamoto

Solubility of silver salicylate in ketones at 25 °C

Solvent	Solubility $10^4 m_1/\text{mol kg}^{-1}$
Acetone	1.35
2-Butanone	0.996
Dipropyl ketone	0.431

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 39 for the binary silver salicylate–methanol system earlier in this section.
Source and Purity of Materials:
The silver salt of salicylic acid was prepared from silver nitrate labeled with radioactive ^{110}Ag and the sodium or potassium salts of the acid.
The solvents were carefully purified.
Estimated Errors:
Solubility: Relative accuracy is 1%–3% at a confidence limit of 0.95.
Temperature: Precision of ±0.5 °C.

2.3.3. 2-Hydroxybenzoic acid salt (NH_4)

Components: (1) Benzoic acid, 2-hydroxy-, monoammonium salt (ammonium salicylate); $C_7H_9NO_3$; [528-94-9] (2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]	**Original Measurements:** [37]H. Henstock, J. Chem. Soc. **1934**, 1340.
Variables: $t/°C=15$	**Prepared by:** H. Miyamoto

Solubility of ammonium salicylate in acetone at 15 °C

Solubility		
Original data[a]	w_1[b] (compiler)	$m_1/\text{mol kg}^{-1}$ (compiler)
69.65	0.4105	4.489

[a] The solubility was originally reported as grams of ammonium salicylate per 100 g of solvent.
[b] $w_1=m_1/\Sigma m_i$, where w_1 is the mass fraction of sodium salicylate. m_1 and Σm_i are the mass of sodium salicylate and mass of solution, respectively.

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 37 for the binary sodium salicylate–methanol system in Sec. 2.3.1.
Source and Purity of Materials:
Ammonium salicylate was recrystallized from boiling methanol.
Acetone was purified by way of its sodium iodide compound, dried over calcium chloride and redistilled; b.p. 56.2 °C at 759 mmHg.
Estimated Errors:
Solubility: Accuracy of 1%.
Temperature: Precision of ±0.1 °C.

2.3.4. 4-Hydroxybenzoic acid salt (Ag)

Components: (1) Benzoic acid, 4-hydroxy-, monosilver salt (silver 4-hydroxybenzoate); $C_7H_5O_3Ag$; [ ] (2) Alcohols: Methyl alcohol (methanol); CH_4O; [67-56-1] Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]	**Original Measurements:** [39]N.A. Izmailov and V.S. Chernyi, Zh. Fiz. Khim. **34**, 319 (1960) [Russ. J. Phys. Chem. (Engl. Transl.) **34**, 149 (1960)].
Variables: $t/°C=25$	**Prepared by:** H. Miyamoto and A. Goto

Solubility of silver 4-hydroxybenzoate in alcohols at 25 °C

Solvent	Solubility $10^3 m_1/\text{mol kg}^{-1}$
Methanol	1.51
Ethanol	0.371

Auxiliary Information

Methods/Apparatus/Procedure:
The experimental details are given in the compilation of Ref. 39 for the binary silver salicylate–methanol system in Sec. 2.3.2.
Source and Purity of Materials:
The silver salt of 4-hydroxybenzoic acid was prepared from silver nitrate labeled with radioactive ^{110}Ag and the sodium or potassium salts of the acid.
The solvents were carefully purified.
Estimated Errors:
Solubility: Relative accuracy is 1%–3% at a confidence limit of 0.95.
Temperature: Precision of ±0.5 °C.

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3. Hydroxybenzoic Acids and Parabens in Ternary Nonaqueous Systems

3.1. Hydroxybenzoic acid and paraben–organic compound (1)–organic compound (2) systems

3.1.1. Salicylic acid

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Benzene; C_6H_6; [71-43-2]
(3) Second component of organic solvent:
Methyl alcohol (methanol); CH_4O; [67-56-1]
Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]
1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]
2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]
Ethanol, 2-ethoxy- (2-ethoxyethanol, ethyl cellosolve); $C_4H_{10}O_2$; [110-80-5]

Original Measurements:

[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).

Variables:

$t/°C=30.6$

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in benzene–alcohol mixtures at 30.6 °C

		Solubility[b]	
Solvent system	Dielectric constant[a]	$\gamma_1/\mathrm{g\ dm^{-3}}$ (compiler)	$c_1/\mathrm{mol\ dm^{-3}}$ (compiler)
Benzene	2.2	7	0.05
Benzene–methanol	16.0	390	2.82
Benzene–ethanol	15.8	430	3.11
Benzene–1-propanol	15.3	315	2.28
Benzene–ethyl cellosolve	14.5	425	3.08
Benzene–2-propanone (acetone)	15.6	510	2.69

[a] The dielectric constant of the solvent mixtures at the maximum solubility of salicylic acid.

[b] In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvents were purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]
(3) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[40]J.W. Marden and M.V. Dover, J. Am. Chem. Soc. **39**, 1 (1917).

Variables:

Concentration of acetone
$t/°C=25$

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in acetone–benzene mixtures at 25 °C

Concentration of acetone		Solubility[a]		
$100w_2$	$100x_2$ (compiler)	Original data	$100w_1$ (compiler)	$m_1/\mathrm{mol\ kg^{-1}}$ (compiler)
100	100.0	55.5	35.7	4.02
90	92.3	51.1	33.8	3.70
80	84.3	46.4	31.7	3.36
70	75.8	(42.3)	29.7	3.06
60	64.7	36.7	26.8	2.66
50	57.4	(31.0)	23.7	2.24
40	47.3	25.3	20.2	1.83
30	36.6	(20.0)	16.7	1.45
20	25.2	15.0	13.0	1.08
10	13.0	7.1	6.6	0.51
0	0.0	0.92	0.91	0.067

[a] In the original paper, the solubility was given as grams per 100 g of the mixed solvent. The values enclosed in parentheses were taken from the curve by the authors.

Auxiliary Information

Methods/Apparatus/Procedure:

The solvents, with a large excess of solid salicylic acid, were shaken in a thermostat for 8–12 h at 25 °C. The solutions were forced out of the bottles through glass wool filters into a weighing pipet, from which the solutions were weighed directly into small glass evaporating dishes and dried on a steam bath and in sulfuric acid desiccators.

Source and Purity of Materials:

Salicylic acid was completely volatilized on heating, leaving no weighable residue. The melting point of the purified acid was 126 °C.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Acetic acid, ethyl ester (ethyl acetate); $C_4H_8O_2$; [141-78-6]
(3) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[40]J.W. Marden and M.V. Dover, J. Am. Chem. Soc. **39**, 1 (1917).

Variables:

Concentration of ethyl acetate
$t/°C=25$

Prepared by:

H. Miyamoto and A. Goto

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Solubility of salicylic acid in ethyl acetate–benzene mixtures at 25 °C

Concentration of ethyl acetate		Solubility[a]		
$100w_2$	$100x_2$ (compiler)	Original data	$100w_1$ (compiler)	m_1/mol kg^{-1} (compiler)
100	100.0	38.0	27.5	2.75
90	88.9	24.2	19.5	1.75
80	78.0	22.7	18.5	1.64
70	67.4	(19.5)	16.3	1.41
60	57.1	16.6	14.2	1.20
50	47.0	(14.5)	12.7	1.05
40	37.1	12.8	11.3	0.927
30	27.5	(9.6)	8.8	0.695
20	18.1	6.2	5.8	0.449
10	9.0	3.42	3.3	0.248
0	0.0	0.92	0.91	0.067

[a] In the original paper, the solubility was given as grams per 100 g of the mixed solvent. The values enclosed in parentheses were taken from the curve by the authors.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 40 for the ternary salicylic acid–acetone–benzene system earlier in this section.

Source and Purity of Materials:

Salicylic acid was completely volatilized on heating, leaving no weighable residue.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid 2-hydroxy- (o-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Methane, tetrachloro- (tetrachloromethane, carbon tetrachloride); CCl_4; [56-23-5]
(3) Benzene; C_6H_6; [71-43-2]

Original Measurements:

[41] W. Herz and M. Levi, Kolloid Z. **50**, 21 (1930).

Variables:

Concentration of benzene
t/°C=25

Prepared by:

E. Königsberger and L.-C. Königsberger

Solubility of salicylic acid in benzene–tetrachloromethane mixtures at 25 °C

Concentration of benzene	Solubility
φ_2	c_1/mmol dm^{-3}
100	50.0
80	47.3
60	44.9
40	42.2
20	37.1
0	29.7

Auxiliary Information

Methods/Apparatus/Procedure:

The solubility of salicylic acid was determined according to the method of Herz and Lorenz [W. Herz and L. Lorenz, Kolloid Z. **47**, 331 (1929)]. Concentrations of saturated solutions were determined by a titrimetric method.

Source and Purity of Materials:

"Best commercial quality" of salicylic acid was purified by recrystallization.

Estimated Errors:

Not stated.

Components:

(1) Benzoic acid, 2-hydroxy- (o-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) 2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one (1,5-dimethyl-2-phenylpyrazol-3-one, antipyrine); $C_{11}H_{12}N_2O$; [60-80-0]
(3) Gasoline

Original Measurements:

[42] I.L. Krupatkin, Zh. Obsh. Khim. **25**, 2189 (1955) [J. Gen. Chem. USSR (Engl. Transl.) **25**, 2151 (1955)].

Variables:

t/°C=76.0–178.0
Composition

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in antipyrine–gasoline mixtures

	Composition of saturated solutions			Demixing temperature
	Salicylic acid	Antipyrine	Gasoline	
Section number	$100w_1$ (compiler)	$100w_2$ (compiler)	$100w_3$	t/°C
1 Salicylic acid 15% Antipyrine 85%	13.95	79.05	7.00	86.0
	13.37	75.40	10.90	117.0
	13.20	74.80	12.00	128.0
	12.02	68.09	19.90	164.0
	2.10	11.90	86.00	162.0
	1.50	8.50	90.00	149.0
	0.75	4.25	95.00	114.0
	0.45	2.55	97.00	96.0
2 Salicylic acid 30% Antipyrine 70%	27.75	64.75	7.50	84.0
	27.00	63.00	10.00	111.0
	25.50	59.50	15.00	145.0
	24.60	57.40	18.00	161.0
	3.60	8.40	88.00	159.0
	2.40	5.60	9.20	134.0
	1.50	3.50	9.60	120.0
	0.90	2.10	9.70	99.0
3 Salicylic acid 43% Antipyrine 57%	40.21	53.30	6.50	76.0
	39.17	51.93	8.90	100.0
	38.70	51.30	10.00	111.0
	36.55	48.45	15.00	139.0
	34.40	45.60	20.00	160.0
	4.30	5.70	90.00	159.0
	2.15	2.85	95.00	125.0
	1.29	1.71	97.00	94.0

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Solubility of salicylic acid in antipyrine–gasoline mixtures

	Composition of saturated solutions			Demixing temperature
	Salicylic acid	Antipyrine	Gasoline	
Section number	100w_1 (compiler)	100w_2 (compiler)	100w_3	t/°C
4 Salicylic acid 50% Antipyrine 50%	46.25	46.25	7.50	84.0
	45.00	45.00	10.00	102.0
	43.40	43.40	13.20	138.0
	40.50	40.50	19.00	163.0
	5.00	5.00	90.00	155.0
	2.50	2.50	95.00	117.0
	2.00	2.00	96.00	114.0
	1.50	1.50	97.00	98.0
5 Salicylic acid 60% Antipyrine 40%	55.20	36.80	8.00	85.0
	54.00	36.00	10.00	100.0
	53.22	35.48	11.30	110.0
	51.00	34.00	15.00	135.0
	48.00	32.00	20.00	160.0
	6.00	4.00	90.00	156.0
	3.00	2.00	95.00	121.0
	1.80	1.20	97.00	96.0
6 Salicylic acid 70% Antipyrine 30%	60.90	26.10	13.00	95.0
	59.50	25.50	15.00	120.0
	56.00	24.00	20.00	145.0
	53.90	23.10	23.00	154.0
	51.10	21.90	27.00	162.0
	14.00	6.00	80.00	178.0
	7.00	3.00	90.00	154.0
	3.50	1.50	95.00	120.0
	2.10	0.90	97.00	98.0
7 Salicylic acid 80% Antipyrine 20%	63.20	15.8	21.00	99.0
	62.40	15.6	22.00	109.0
	60.00	15.0	25.00	122.0
	56.00	14.0	30.00	130.0
	52.00	13.0	35.00	149.0
	41.12	10.28	48.60	151.5
	36.00	9.00	55.00	154.0
	28.00	7.30	65.00	163.0
	20.00	5.00	75.00	163.0
	16.00	4.00	80.00	152.0
	12.00	3.00	85.00	139.0
	8.00	2.00	90.00	123.0
	4.80	1.20	94.00	109.0
8 Salicylic acid 90% Antipyrine 10%	49.50	5.00	45.00	95.0
	45.00	5.00	50.00	110.0
	36.00	4.00	60.00	123.0
	27.00	3.00	70.00	128.0
	18.00	2.00	80.00	132.0
	13.50	1.50	85.00	125.0
	9.00	1.00	90.00	103.0

Auxiliary Information

Methods/Apparatus/Procedure:

The experiment was performed by the polythermic method in sealed glass ampoules. The three-component system was studied by polythermic sections through their prisms taken from the edge for gasoline to the plane for the binary system antipyrine–salicylic acid.

Source and Purity of Materials:

Pharmaceutical antipyrine and chemically pure grade salicylic acid were used.

A gasoline fraction boiling in the 120–140 °C range was used.

Estimated Errors:

Nothing specified.

Components:

(1) Benzoic acid, 2-hydroxy- (o-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]

(2) Acetic acid, ethyl ester (ethyl acetate); $C_4H_8O_2$; [141-78-6]

(3) Second component of organic solvent:

Methyl alcohol (methanol); CH_4O; [67-56-1]

Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Ethanol, 2-ethoxy- (2-ethoxyethanol, ethyl cellosolve); $C_4H_{10}O_2$; [110-80-5]

2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

1,2-Propanediol (propane-1,2-diol, propylene glycol); $C_3H_8O_2$; [57-55-6]

Original Measurements:

[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).

Variables:

t/°C=30.6

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in ethyl acetate–alcohol mixtures at 30.6 °C

		Solubility[b]	
Solvent system	Dielectric constant[a]	γ_1/g dm^{-3} (compiler)	c_1/mol dm^{-3} (compiler)
Ethyl acetate	6.0	23	0.17
Ethyl acetate–methanol	16.0	335	2.43
Ethyl acetate–ethanol	15.7	390	2.82
Ethyl acetate–1-propanol (n-propanol)	15.3	355	2.57
Ethyl acetate–1-butanol (n-butanol)	14.0	330	2.39
Ethyl acetate–ethanol, 2-ethoxy- (ethyl cellosolve)	14.5	425	3.08
Ethyl acetate–2-propanone (acetone)	16.1	415	3.00
Ethyl acetate–1,2-propanediol (propylene glycol)	16.2	160	1.16

[a]The dielectric constant of the binary mixtures at the maximum solubility of salicylic acid.

[b]In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials

The solvents were purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

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Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]

(2) Chloroform; $CHCl_3$; [67-66-3]

(3) Second component of organic solvent:

Methyl alcohol (methanol); CH_4O; [67-56-1]

Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Ethanol, 2-ethoxy- (2-ethoxyethanol, ethyl cellosolve); $C_4H_{10}O_2$; [110-80-5]

2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

1,2-Propanediol (propane-1,2-diol, propylene glycol); $C_3H_8O_2$; [57-55-6]

Original Measurements:

[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).

Variables:

t/ °C=30.6

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in chloroform–alcohol mixtures at 30.6 °C

Solvent system	Dielectric constant[a]	Solubility[b] γ_1 / g dm^{-3} (compiler)	c_1 / mol dm^{-3} (compiler)
Chloroform	4.8	2	0.014
Chloroform–methanol	16.0	348	2.52
Chloroform–ethanol	15.7	595	4.31
Chloroform–1-propanol	15.3	315	2.28
Chloroform–1-butanol	14.0	425	2.04
Chloroform–ethyl cellosolve	14.5	425	3.08
Chloroform–acetone	16.1	445	3.22
Chloroform–propylene glycol	15.2	292	2.11

[a]The dielectric constant of the binary mixtures at the maximum solubility of salicylic acid.

[b]In the original paper, the solubility was given as mg/ml of solution.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvents were purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

(3) Second component of organic solvent:

Methyl alcohol (methanol); CH_4O; [67-56-1]

Ethyl alcohol (ethanol); C_2H_6O; [64-17-5]

1-Propanol (propan-1-ol, propyl alcohol); C_3H_8O; [71-23-8]

1-Butanol (butan-1-ol, butyl alcohol); $C_4H_{10}O$; [71-36-3]

Ethanol, 2-ethoxy- (2-ethoxyethanol, ethyl cellosolve); $C_4H_{10}O_2$; [110-80-5]

2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

1,2-Ethanediol (ethane-1,2-diol, ethylene glycol); $C_2H_6O_2$; [107-21-1]

1,2-Propanediol (propane-1,2-diol, propylene glycol); $C_3H_8O_2$; [57-55-6]

Original Measurements:

[17]A.N. Paruta, B.J. Sciarrone, and N.G. Lordi, J. Pharm. Sci. **53**, 1349 (1964).

Variables:

t/ °C=30.6

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in dioxane–alcohols mixtures at 30.6 °C

Solvent system	Dielectric constant[a]	Solubility[b] γ_1 / g dm^{-3} (compiler)	c_1 / mol dm^{-3} (compiler)
1,4-Dioxane	2.2	40	0.29
1,4-Dioxane–methanol	16.3	440	3.19
1,4-Dioxane–ethanol	15.0	495	3.58
1,4-Dioxane–propanol	14.8	305	2.21
1,4-Dioxane–1-butanol	14.5	268	1.94
1,4-Dioxane–ethyl cellosolve	14.5	425	3.08
1,4-Dioxane–acetone	15.6	475	3.44
1,4-Dioxane–ethylene glycol	17.5	89	0.64
1,4-Dioxane–propylene glycol	15.1	290	2.10

[a]The dielectric constant of the solvent mixtures at the maximum solubility of salicylic acid.

[b]In the original paper, the solubility was given as mg/ml of solution.

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 17 for the salicylic acid–ethanol system in Sec. 2.1.2.1.

Source and Purity of Materials:

The solvents were purified by the method described in A. Weissberger *et al.*, *Organic Solvents*, 2nd ed. (Interscience, New York, 1955), Chaps. 4 and 5.

Estimated Errors:

Solubility: Nothing specified.

Temperature: Precision of ±0.2 °C (solubility) and ±1.0 °C (dielectric constant).

3.1.2. Methylparaben

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, methyl ester (methyl 4-hydroxybenzoate, methylparaben); $C_8H_8O_3$; [99-76-3] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5] (3) Cyclohexane; C_6H_{12}; [110-82-7]	[43]R.H. Manzo and A.A. Ahumada, J. Pharm. Sci. **79**, 1109 (1990).
Variables:	**Prepared by:**
Concentration of cyclohexane $t/{}^\circ C = 15-50$	A. Goto and R. Goto

Solubility of methylparaben in ethanol–cyclohexane mixtures

Temperature	Concentration of cyclohexane	Solubility
$t/{}^\circ C$	$100\varphi_3$	$10^3 x_3$
15	100	0.0441
	96	6.85
	92	15.9
	83	32.4
25	100	0.0726
	96	8.33
	92	19.4
	85	42.9
40	100	0.247
	96	13.3
	92	30.8
	85	62.6
50	100	0.425
	96	18.0
	92	41.2
	85	75.0

Auxiliary Information

Methods/Apparatus/Procedure:

Solvent mixtures were prepared by mixing exactly measured volumes of absolute ethanol and cyclohexane. A suitable amount of solvent was introduced into a stoppered test tube containing an excess amount of solute, and was kept at least 24 h in a constant-temperature bath with adequate shaking. Samples were taken with a small diameter tube having a piece of sintered glass in its end to avoid contamination with the solid. Pipettes and filter devices were previously heated in an oven to reach the same temperature as that of the experiment. The ester concentration was determined spectrophotometrically.

Source and Purity of Materials:

Methylparaben was obtained from Aldrich and purified by recrystallization, m.p. 398.4 K [R.H. Manzo, A.A. Ahumada, and E. Luna, J. Pharm. Sci. **73**, 1094 (1984); R.H. Manzo, A.A. Ahumada, and E. Luna, J. Pharm. Sci. **73**, 1869 (1984)].

Ethanol was analytical grade obtained from Merck.

Cyclohexane (analytical grade) was obtained from Mallinckrodt.

Estimated Errors:

Nothing specified.

3.1.3. Propylparaben

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy-, propyl ester (propyl *p*-hydroxybenzoate, propylparaben); $C_{10}H_{12}O_3$; [94-13-3] (2) Ethyl alcohol (ethanol); C_2H_6O; [64-17-5] (3) Cyclohexane; C_6H_{12}; [110-82-7]	[43]R.H. Manzo and A.A. Ahumada, J. Pharm. Sci. **79**, 1109 (1990).
Variables:	**Prepared by:**
Concentration of cyclohexane $t/{}^\circ C = 15-50$	A. Goto and R. Goto

Solubility of propylparaben in ethanol–cyclohexane mixtures

Temperature	Concentration of cyclohexane	Solubility
$t/{}^\circ C$	$100\varphi_3$	$10^3 x_1$
15	100	0.0944
	96	17.0
	92	38.1
	83	68.3
25	100	0.224
	96	23.8
	92	46.8
	85	91.3
40	100	0.682
	96	43.4
	92	92.9
	85	155
50	100	1.59
	96	64.8
	92	171
	85	249

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Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 43 for the methylparaben–ethanol–cyclohexane system in Sec. 3.1.2.

Source and Purity of Materials:

Propylparaben was obtained from Aldrich and purified by recrystallization, m.p. 369.2 K [R.H. Manzo, A.A. Ahumada, and E. Luna, J. Pharm. Sci. **73**, 1094 (1984); R.H. Manzo, A.A. Ahumada, and E. Luna, J. Pharm. Sci. **73**, 1869 (1984)].

Ethanol was analytical grade obtained from Merck.

Cyclohexane (analytical grade) was obtained from Mallinckrodt.

Estimated Errors:

Nothing specified.

3.2. Hydroxybenzoic acid–organic compound–inorganic compound systems

3.2.1. Salicylic acid

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9]
(3) Methyl alcohol (methanol); CH_4O; [67-56-1]

Original Measurements:

[44]G.S. Gurdial, S.J. Macnaughton, D.L. Tomasko, and N.R. Foster, Ind. Eng. Chem. Res. **32**, 1488 (1993).

Variables:

T/K=318.2, 323.2, and 328.2
Pressure: 91–201×10^5 Pa

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in supercritical carbon dioxide–methanol (3.5 mol %) mixture

Temperature T/K	Pressure[a] 10^5 Pa	Density ρ/g dm^{-3}	Solubility[b] 10^3x_1
318.2	96	432.3	1.25
	101	514.1	1.62
	111	611.5	2.49
	121	663.4	2.97
	131	697.9	3.28
	141	724.0	3.51
	161	762.6	3.93
	181	791.4	4.26
	201	814.5	4.48
323.2	101	397.3	1.21
	111	514.4	2.11
	121	592.5	2.68
	141	676.6	3.59
	161	725.1	4.07
	201	786.3	4.76
328.2	101	333.3	1.12
	111	425.5	1.66
	121	513.9	2.52
	141	623.9	3.64
	161	684.7	4.28
	201	756.8	5.12

[a] In the original paper, the pressure was given as "bar." 1 bar=10^5 Pa.
[b] 3.5 mol % cosolvent concentration on a solute-free basis.

Auxiliary Information

Methods/Apparatus/Procedure:

The solubilities were determined using a continuous flow apparatus [G.S. Gurdial and N.R. Foster, Ind. Eng. Chem. Res. **30**, 575 (1991)]. The high-pressure liquid chromatography pump was replaced with a high-pressure syringe pump to facilitate preparation of the CO_2-cosolvent mixtures.

The binary mixtures of CO_2 with methanol were prepared directly by loading a high-pressure syringe pump with a known volume of the organic solvent and then adding the liquid CO_2 at about 50 bar. The total volume of the syringe pump was 260 ± 5 cm^3. The pump was calibrated with N_2 gas at various pressures. To facilitate the flow of liquid CO_2 from the cylinder to the syringe pump, a cooling jacket was installed around the barrel of the syringe. Cooling water at approximately 274 K was recirculating through the jacket with a magnetic pump during the preparation stage. The temperature of the recirculating water was determined with a thermometer located at the exit of the cooling jacket. The pressure in the syringe pump was adjusted to yield the desired value of CO_2 density. After the solvent mixture was prepared, the contents were heated to approximately 313 K by recirculating warm water in the cooling/heating jacket for duration of 10 min. The contents were cooled to about 280 K for approximately 10 min. The heating and cooling sequence was repeated several times, after which the contents were allowed to further mix and equilibrate for 6 h at ambient temperature.

A given mixture of CO_2–cosolvent was prepared, the equilibrium cells were charged with the binary mixture and the system temperature was raised to the desired value. Extraction of the solid was initially performed at the desired pressure until the entire content of the syringe pump was used. Solubilities were determined at temperatures and pressures above the mixture critical point to ensure operation in the supercritical region. The minimum extraction temperature and pressure used were 318 K and 90 bar, respectively. The solubility measurements in these ternary systems were determined using the same procedure [G. S. Gurdial and N. R. Foster, Ind. Eng. Chem. Res. **30**, 575 (1991)]. The procedure involved flushing the regulating valve with an organic solvent and measuring the amount of solute deposited in a Petri dish after drying its contents. The amount of solute collected in the 2 mm filter used as a collection device was determined gravimetrically. In order to remove traces of cosolvent, the in-line filter was placed in an oven at a temperature of 318 K for approximately 1 h.

The solubility was determined from the total mass of the solute collected and the total volume of gas measured with a wet test meter at ambient conditions. Each reported data point represents an average of three trials.

Source and Purity of Materials:

Carbon dioxide was purchased from Liquid Air, and the purity was 99.8%.

Methanol was from GDH, and the purity was 99.8%.

Salicylic acid was from Ajax Chemicals, and the purity of the acid was 99.0%.

These materials were used without further purification.

Estimated Errors:

Solubility: Precision less than 5% CO_2.

Pressure: Uncertainty within ±2%.

Temperature: Nothing specified.

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Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9]
(3) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]

Original Measurements:

[44]G.S. Gurdial, S.J. Macnaughton, D.L. Tomasko, and N.R. Foster, Ind. Eng. Chem. Res. **32**, 1488 (1993).

Variables:

$T/\mathrm{K}=318.2$, 323.2, and 328.2
Pressure: $86-201\times10^5$ Pa

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in supercritical carbon dioxide–acetone (3.5 mol %) mixture

Temperature	Pressure[a]	Density	Solubility[b]
T/K	10^5 Pa	$\rho/\mathrm{g\ dm^{-3}}$	10^3x_1
318.2	86	302.4	0.68
	91	352.2	0.80
	101	514.1	1.25
	111	611.5	1.48
	121	663.4	1.72
	141	724.0	1.85
	161	762.6	1.94
	201	814.5	2.10
323.2	91	293.2	0.72
	96	340.2	0.83
	101	397.3	1.09
	111	514.4	1.46
	121	592.5	1.70
	141	676.6	2.02
	161	725.1	2.13
	201	786.3	2.33
328.2	101	333.3	0.93
	111	425.5	1.22
	121	513.9	1.54
	141	623.9	2.10
	161	684.7	2.33
	201	756.8	2.52

[a] In the original paper, the pressure was given as "bar." 1 bar$=10^5$ Pa.
[b] 3.5 mol % cosolvent concentration on a solute-free basis.

Auxiliary Information

Methods/Apparatus/Procedure

The experimental details are given in the compilation of Ref. 44 for the salicylic acid–carbon dioxide (supercritical)–methanol system earlier in this section.

Source and Purity of Materials:

Carbon dioxide was purchased from Liquid Air, and the purity was 99.8%.

Acetone was from BDH, and the purity was 99.5%.

Salicylic acid was from Ajax Chemicals and the purity of the acid was 99.0%.

These materials were used without further purification.

Estimated Errors:

Solubility: Precision less than 5%.

CO_2 pressure: Uncertainty within ±2% (relative).

Temperature: Nothing specified.

Components:

(1) Benzoic acid, 2-hydroxy- (*o*-hydroxybenzoic acid, salicylic acid); $C_7H_6O_3$; [69-72-7]
(2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9]
(3) Acetic acid, ethyl ester (ethyl acetate); $C_4H_8O_2$; [141-78-6]

Original Measurements:

[45]Z. Liu, D. Li, G. Yang, and B. Han, J. Supercrit. Fluids **18**, 111 (2000).

Variables:

Concentration of CO_2
$T/\mathrm{K}=308.15$ and 318.15
$p/\mathrm{MPa}=2.22-8.02$

Prepared by:

H. Miyamoto and A. Goto

Solubility of salicylic acid in supercritical carbon dioxide–ethyl acetate mixtures

Temperature	Pressure	Concentration of CO_2	Solubility	Molar volume of the liquid solution
T/K	MPa	x_2	x_1	$V_\mathrm{m}(\mathrm{ml/mol})$
308.15	2.22	0.3502	0.091 8	79.9
	3.01	0.4548	0.070 7	73.5
	3.54	0.5231	0.049 6	70.3
	4.02	0.5992	0.038 5	67.4
	4.35	0.6381	0.032 3	65.8
	4.63	0.6750	0.025 2	64.5
	4.90	0.7265	0.019 8	63.6
	5.40	0.7895	0.011 8	62.5
	5.93	0.8581	0.006 27	59.0
	6.32	0.8939	0.003 84	58.8
	6.68	0.9140	0.001 19	61.2
318.15	2.51	0.3498	0.099 8	81.1
	3.07	0.4177	0.086 1	77.6
	3.41	0.4549	0.072 6	74.9
	4.16	0.5366	0.058 3	69.4
	4.79	0.6087	0.038 2	66.1
	5.32	0.6646	0.029 6	68.1
	5.56	0.6825	0.024 2	65.9

Auxiliary Information

Methods/Apparatus/Procedure:

The apparatus for determining the solubility of a solute in a liquid solvent expanded with high-pressure gas or supercritical fluid was used. It is mainly composed of a gas cylinder, a high-pressure syringe pump, a solenoid-operated circulating pump, a liquid sample bomb, a view cell, a pressure gauge, a constant-temperature bath, and valves and fitting of different kinds. All metallic parts in direct contact with the chemicals were made of stainless steel (the experimental setup was shown in the paper). The volume of the view cell in which the liquid solution was allowed to contact with antisolvent carbon dioxide was about 200 ml. The solenoid-operated pump was used to circulate the vapor phase in order to equilibrate the system quickly. The system pressure was monitored through the pressure gauge, which was composed of a transducer and an indicator.

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The ethyl acetate solution saturated with a solute at ambient temperature was sucked into the view cell by evacuating the system. After thermal equilibrium was reached, carbon dioxide was charged into the system until the desired pressure was reached. The solenoid-operated pump was started to circulate the vapor phase through valve V4 and the bottom of the view cell. All experiments were conducted with V-L-S three phases. After the pressure and the vapor-liquid interface had been unchanged for 2 h, the solid-liquid-vapor equilibrium was considered reached. The solenoid-operated pump was stopped and the system was maintained at static conditions to allow the solid to deposit until the solution became completely clear. Then valves V3 and V7 were opened. The liquid solution in the view cell began to flow into the sample bomb to replace the vapor in it, which resulted from hydraulic pressure. When the vapor-liquid interface in the view cell was the same as that in the V3, V5, V6, V8, V7 loop, it remained unchanged with time. At this time, the liquid sample bomb was full of liquid solution. Valves (V5–V8) were closed and the sample bomb was removed for composition analysis.

The mass of the sample in the sample bomb was determined by a balance. The sample bomb was connected to an analysis system. The experimental setup consisted of a pressure gauge, liquid sample bomb, flush vessel, and constant-temperature bath (the experimental setup was shown in the paper). Then the apparatus was put into ice water. After evacuating the system, the solution in the sample bomb was flushed into the vessel and vapor-liquid equilibrium was reached at low pressure (<0.5 MPa). The amount of carbon dioxide in the vapor phase was calculated from the Huang equation of state on the basis of the pressure, temperature, volume of the system, and the saturated vapor pressure of ethyl acetate. The amount of carbon dioxide in the liquid phase was relatively small and was estimated from a solubility versus pressure curve in the pressure range from 0 to 0.5 MPa at the analysis temperature, which was determined experimentally in this study. The solute in the analysis system was washed into a beaker using ethyl acetate and dried and its mass was determined gravimetrically. The amount of the ethyl acetate in the sample was known from the total mass of the sample, the mass of carbon dioxide, and the mass of the solute. Thus, the moles of the three components were calculated. From the volume of the sample bomb and the total moles of the three components, the molar volumes of the mixture were easily obtained.

Source and Purity of Materials:

Carbon dioxide with a purity of 99.95% was supplied by Haunxin Gas Company.

Beijing Chemical Reagent Plant supplied ethyl acetate with a purity of 99.9%.

Salicylic acid with purity of 99.9% was purchased from Beijing Chemical Reagent Plant, and was not purified further.

Estimated Errors:

The accuracy of the pressure gauge was ±0.025 MPa in the pressure range 0–20 MPa.

The accuracy of the temperature was within ±0.1 K.

The accuracy of the method for the amount of carbon dioxide was better than ±0.5%.

The accuracy of the solute mass was ±0.2%.

3.2.2. 3-Hydroxybenzoic acid

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9] (3) Methyl alcohol (methanol); CH_4O; [67-56-1]	[44]G.S. Gurdial, S.J. Macnaughton, D.L. Tomasko, and N.R. Foster, Ind. Eng. Chem. Res. **32**, 1488 (1993).

Variables:	**Prepared by:**
$T/\mathrm{K}=318.2$, 323.2, and 328.2 Pressure: $91-201\times10^5$ Pa	H. Miyamoto and A. Goto

Solubility of 3-hydroxybenzoic acid in supercritical carbon dioxide–methanol (3.5 mol %) mixture

Temperature	Pressure[a]	Density	Solubility[b]
T/K	10^5 Pa	$\rho/\mathrm{g\ dm^{-3}}$	10^5x_1
318.2	91	352.2	1.59
	101	514.1	2.63
	111	611.5	3.07
	121	663.4	3.26
	141	724.0	3.49
	161	762.6	3.76
	201	814.5	3.99
323.2	101	397.3	2.04
	111	514.4	2.81
	121	592.5	3.22
	141	676.6	3.59
	161	725.1	3.98
	201	786.3	4.19
328.2	101	333.3	1.78
	111	425.5	2.65
	121	513.9	3.18
	141	623.9	3.86

[a] In the original paper, the pressure was given as "bar." 1 bar$=10^5$ Pa.

[b] 3.5 mol % cosolvent concentration on a solute-free basis.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 44 for the salicylic acid–carbon dioxide (supercritical)–methanol system in Sec. 3.2.1.

Source and Purity of Materials:

Carbon dioxide was purchased from Liquid Air, and the purity was 99.8%.

Methanol was from BDH, and the purity was 99.8%.

3-Hydroxybenzoic acid was from BDH and the purity of the acid was 99.0%.

These materials were used without further purification.

Estimated Errors:

Solubility: Precision less than 5%.

CO_2 pressure: Uncertainty within ±2%.

Temperature: Nothing specified.

Components:	**Original Measurements:**
(1) Benzoic acid, 3-hydroxy- (*m*-hydroxybenzoic acid); $C_7H_6O_3$; [99-06-9] (2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9] (3) 2-Propanone (propan-2-one, acetone); C_3H_6O; [67-64-1]	[44]G.S. Gurdial, S.J. Macnaughton, D.L. Tomasko, and N.R. Foster, Ind. Eng. Chem. Res. **32**, 1488 (1993).

Variables:	**Prepared by:**
$T/\mathrm{K}=318.2$, 323.2, and 328.2 Pressure: $86-201\times10^5$ Pa	H. Miyamoto and A. Goto

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Solubility of 3-hydroxybenzoic acid in supercritical carbon dioxide–acetone (3.5 mol %) mixture

Temperature	Pressure[a]	Density	Solubility[b]
T/K	10^5 Pa	$\rho/\mathrm{g\ dm^{-3}}$	$10^5 x_1$
318.2	91	352.2	1.50
	101	514.1	2.56
	111	611.5	3.26
	121	663.4	3.73
	141	724.0	4.28
	161	762.6	4.49
	181	791.4	4.58
	201	814.5	4.83
323.2	96	340.2	1.67
	106	459.0	2.47
	111	514.4	2.85
	121	592.5	3.36
	141	676.6	4.37
	161	725.1	4.72
	201	786.3	5.16
328.2	101	333.3	1.77
	111	425.5	2.40
	121	513.9	3.14
	131	578.4	3.95
	141	623.9	4.45

[a] In the original paper, the pressure was given as "bar." 1 bar $=10^5$ Pa.

[b] 3.5 mol % cosolvent concentration on a solute-free basis.

Auxiliary Information

Methods/Apparatus/Procedure:

The experimental details are given in the compilation of Ref. 44 for the salicylic acid–carbon dioxide–methanol system in Sec. 3.2.1.

Source and Purity of Materials:

Carbon dioxide was purchased from Liquid Air, and the purity was 99.8%.

Acetone was from BDH, and the purity was 99.5%.

3-Hydroxybenzoic acid was from BDH and the purity of the acid was 99.0%.

These materials were used without further purification.

Estimated Errors:

Solubility: Precision less than 5%.

CO_2 pressure: Uncertainty within ±2%.

Temperature: Nothing specified.

3.2.3. 4-Hydroxybenzoic acid

Components:	**Original Measurements:**
(1) Benzoic acid, 4-hydroxy- (*p*-hydroxybenzoic acid); $C_7H_6O_3$; [99-96-7] (2) Carbon dioxide (supercritical fluid); CO_2; [124-38-9] (3) Acetic acid, ethyl ester (ethyl acetate); $C_4H_8O_2$; [141-78-6]	[45] Z. Liu, D. Li, G. Yang, and B. Han, J. Supercrit. Fluids **18**, 111 (2000).
Variables:	**Prepared by:**
Concentration of CO_2 $T/\mathrm{K}=308.15$ and 318.15 $p/\mathrm{MPa}=2.33-8.18$	H. Miyamoto and A. Goto

Solubility of 4-hydroxybenzoic acid in supercritical carbon dioxide–ethyl acetate mixtures

Temperature	Pressure	Concentration of CO_2	Solubility	Molar volume of the liquid solution
T/K	MPa	x_2	x_1	V_m(ml/mol)
308.15	2.33	0.3871	0.024 9	78.7
	2.57	0.4323	0.021 6	73.6
	2.97	0.4724	0.018 0	73.9
	3.05	0.5090	0.015 5	71.8
	4.08	0.6394	0.010 6	64.7
	4.59	0.6957	0.006 67	63.7
	5.17	0.7862	0.002 92	59.0
	5.80	0.8374	0.001 69	58.7
	6.66	0.9063	0.000 30	57.0
	6.78	0.9397	0.000 17	56.2
	6.96	0.9528	0.000 070	56.0
318.15	2.58	0.3544	0.032 5	80.7
	3.74	0.5055	0.018 2	72.5
	5.05	0.6377	0.012 8	67.4
	5.21	0.6753	0.009 46	59.1
	5.94	0.7423	0.005 64	60.0
	6.72	0.8251	0.003 51	63.4
	7.58	0.9037	0.000 55	62.2
	7.91	0.9175	0.000 21	62.0
	8.00	0.9404	0.000 082	60.6
	8.18	0.9546	0.000 013	59.0

Auxiliary Information

Methods/Apparatus/Procedure:

The apparatus and procedure for determining the solubility of 4-hydroxybenzoic acid in supercritical carbon dioxide with ethyl acetate were identical with that used for the solubility determination of salicylic acid in supercritical carbon dioxide with ethyl acetate; see the compilation of Ref. 45 in Sec. 3.2.1.

Source and Purity of Materials:

Carbon dioxide with a purity of 99.95% was supplied by Haunxin Gas Company.

Beijing Chemical Reagent Plant supplied ethyl acetate with a purity of 99.9%.

4-Hydroxybenzoic acid with purity of 99.9% was purchased from Beijing Chemical Reagent Plant, and was not purified further.

Estimated Errors:

The accuracy of the pressure gauge was ±0.025 MPa in the pressure range 0–20 MPa.

The accuracy of the temperature was within ±0.1 K.

The accuracy of the method for the amount of carbon dioxide was better than ±0.5%.

The accuracy of the solute mass was ±0.2%.

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