IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 9. C_{10} Hydrocarbons with Water

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The mutual solubilities and related liquid–liquid equilibria of C_{10} hydrocarbons with water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 20 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For ten systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of the all experimental data for a given homologous series of aliphatic and aromatic hydrocarbons was used. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2131103]

Key words: C_{10} hydrocarbons; critical evaluation; liquid–liquid equilibria; solubilities; water.

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*Deceased. This work is dedicated to his memory.

Contents

*A Critical Evaluation is prepared for the system.

List of Tables

List of Figures

1. Preface

1.1. Scope of this Volume

This paper is Part 9 of a revised and updated version of an earlier compilation and evaluation of the mutual solubilities of water and hydrocarbon compounds containing five or more carbon atoms.[1,2] This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

This revised work also includes all new evaluations for systems where two or more independent measurements of solubility have been reported. In these evaluations reported solubility values are characterized as ''Recommended, Tentative, Doubtful, or Rejected,'' based on consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.[3–8] Recommended values are supported by two (or more) independent experimental values and a reference value that are all in agreement. Tentative values are supported by two (or more) independent values in agreement with each other, but not with the reference value, or one experimental value in agreement with the reference value. Doubtful values are those for which a single experimental value differs from the reference value. Experimental values that differ from reference values and other experimental values are Rejected.

Detailed introductory material including explanations of the formats of compilation and evaluation, definitions of commonly used measures of solubility, and the scope of the Solubility Data Series can be found in Part 1.[7] The derivation of the smoothing equations used for calculate reference values can be found in Parts 1 and 2.[7,8]

1.2. References for the Preface

[1] D. Shaw, Editor, *IUPAC Solubility Data Series, Vol. 37*, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C5 to C7 (Pergamon, New York, 1989).

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2. C_{10} Hydrocarbons with Water

2.1. Naphthalene+Water

Components:	**Evaluators:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of Naphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Akiyoshi *et al.*[1]	298	May *et al.*[13]	298
Andrews and Keefer[2]	298	May *et al.*[14]	281–300
Bennett and Canady[3]	275–318	Mitchell[15]	288–298
Bohon and Claussen[4]	298	Schwarz[17]	282–305
Coyle *et al.*[5]	295	Schwarz and Wasik[18]	285–298
Dickhut *et al.*[6]	298	Schwarz and Wasik[19]	298
Eganhouse and Calder[7]	298	Van Meter and Neumann[20]	298
Gordon and Thorne[8]	298	Vesala[21]	298
Hilpert[9]	273–298	Vesala and Loennberg[22]	298
Janado *et al.*[10]	298	Walters and Luthy[23]	298
Klevens[11]	298	Wauchope and Getzen[24]	273–348
Mackay and Shiu[12]	298		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \tag{1}$$

where: $\ln x_{1,\min} = -13.49$; $D = 67.235$; $T_{\min} = 245$ K (hypothetical).

The parameters $\ln x_{1,\min}$, $T_{\min}$, and D are adjustable constants. The values of these constants were obtained from regression of the experimental data for solubility of naphthalene in water reported in this paper.

Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 1.

All the experimental and reference data are listed in Table 2 and shown in Fig. 1.

High Pressure Solubility of Naphthalene (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by Sawamura *et al.*[16] at 298 K and 45 400–207 300 kPa have not been critically evaluated because the developed method is not applicable for such data.

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[22] A. Vesala and H. Loennberg, Acta Chem. Scand., Ser. A **34**, 187 (1980).
[23] R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
[24] R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

TABLE 1. The data categories for solubility of naphthalene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
273.2		Hilpert,[9] Wauchope and Getzen[24]	
275.1		Bennett and Canady[3]	
281.4		May *et al.*[14]	
281.6		Schwarz[17]	
283.9		Bennett and Canady[3]	
284.3		Schwarz[17]	
284.7		May *et al.*[14]	
285.2		Schwarz and Wasik[18]	
286.6		May *et al.*[14]	
287.2		Schwarz[17]	
288.2		Mitchell[15]	
288.3		May *et al.*[14]	
288.6		Bennett and Canady[3]	
290.7		Schwarz[17]	
291.2		Schwarz and Wasik[18]	
292.5		May *et al.*[14]	
293.4		Schwarz[17]	
294.9		Bennett and Canady[3]	
295.0		Coyle *et al.*[5]	
295.4		Wauchope and Getzen[24]	
296.4		Schwarz[17]	
296.6		May *et al.*[14]	
297.7		Wauchope and Getzen[24]	
298.0		Vesala[21]	
298.1		Gordon and Thorne[8]	

298.2	Akiyoshi *et al.*,[1] Andrews and Keefer,[2] Bohon and Claussen,[4] Dickhut *et al.*,[6] Eganhouse and Calder,[7] Hilpert,[9] Janado *et al.*,[10] Mackay and Shiu,[12] May *et al.*,[13] May *et al.*,[14] Schwarz,[17] Schwarz and Wasik,[18] Van Meter and Neumann,[20] Vesala and Loennberg[22] Walters and Luthy,[23] Wauchope and Getzen[24]	Schwarz and Wasik[19]	Klevens,[11] Mitchell[15]
298.4		Bennett and Canady[3]	
299.5		Schwarz[17]	
300.2		May *et al.*[14]	
302.4		Schwarz[17]	
303.1		Wauchope and Getzen[24]	
303.5		Wauchope and Getzen[24]	
303.9		Bennett and Canady[3]	
305.0		Schwarz[17]	
307.7		Wauchope and Getzen[24]	
308.3		Bennett and Canady[3]	
312.5	Bennett and Canady,[3] Wauchope and Getzen[24]		
313.3		Wauchope and Getzen[24]	
317.9		Wauchope and Getzen[24]	
318.1		Bennett and Canady[3]	
323.2		Wauchope and Getzen[24]	
323.4		Wauchope and Getzen[24]	
328.8		Wauchope and Getzen[24]	
337.7		Wauchope and Getzen[24]	
346.6		Wauchope and Getzen[24]	
348.2		Wauchope and Getzen[24]	

TABLE 2. Experimental values for solubility of naphthalene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$2.7\cdot 10^{-6}$ (T; Ref. 9), $1.930\cdot 10^{-6}$ (T; Ref. 24)	$2.0\cdot 10^{-6}$
275.1	$1.696\cdot 10^{-6}$ (T; Ref. 3)	$2.1\cdot 10^{-6}$
281.4	$2.376\cdot 10^{-6}$ (T; Ref. 14)	$2.5\cdot 10^{-6}$
281.6	$2.521\cdot 10^{-6}$ (T; Ref. 17)	$2.5\cdot 10^{-6}$
283.9	$2.417\cdot 10^{-6}$ (T; Ref. 3)	$2.7\cdot 10^{-6}$
284.3	$2.679\cdot 10^{-6}$ (T; Ref. 17)	$2.7\cdot 10^{-6}$
284.7	$2.703\cdot 10^{-6}$ (T; Ref. 14)	$2.7\cdot 10^{-6}$
285.2	$2.831\cdot 10^{-6}$ (T; Ref. 18)	$2.8\cdot 10^{-6}$
286.6	$2.862\cdot 10^{-6}$ (T; Ref. 14)	$2.9\cdot 10^{-6}$
287.2	$2.991\cdot 10^{-6}$ (T; Ref. 17)	$3.0\cdot 10^{-6}$
288.2	$3.1\cdot 10^{-6}$ (T; Ref. 15)	$3.1\cdot 10^{-6}$
288.3	$3.018\cdot 10^{-6}$ (T; Ref. 14)	$3.1\cdot 10^{-6}$
288.6	$3.042\cdot 10^{-6}$ (T; Ref. 3)	$3.1\cdot 10^{-6}$
290.7	$3.389\cdot 10^{-6}$ (T; Ref. 17)	$3.3\cdot 10^{-6}$
291.2	$3.420\cdot 10^{-6}$ (T; Ref. 18)	$3.4\cdot 10^{-6}$
292.5	$3.624\cdot 10^{-6}$ (T; Ref. 14)	$3.5\cdot 10^{-6}$
293.4	$3.730\cdot 10^{-6}$ (T; Ref. 17)	$3.6\cdot 10^{-6}$
294.9	$3.757\cdot 10^{-6}$ (T; Ref. 3)	$3.8\cdot 10^{-6}$
295.0	$4.77\cdot 10^{-6}$ (T; Ref. 5)	$3.8\cdot 10^{-6}$
295.4	$3.981\cdot 10^{-6}$ (T; Ref. 24)	$3.9\cdot 10^{-6}$
296.4	$4.001\cdot 10^{-6}$ (T; Ref. 17)	$4.0\cdot 10^{-6}$
296.6	$4.143\cdot 10^{-6}$ (T; Ref. 14)	$4.1\cdot 10^{-6}$
297.7	$4.308\cdot 10^{-6}$ (T; Ref. 24)	$4.2\cdot 10^{-6}$
298.0	$4.520\cdot 10^{-6}$ (T; Ref. 21)	$4.3\cdot 10^{-6}$
298.1	$4.719\cdot 10^{-6}$ (T; Ref. 8)	$4.3\cdot 10^{-6}$
298.2	$4.248\cdot 10^{-6}$ (R; Ref. 1), $4.422\cdot 10^{-6}$ (R; Ref. 2), $4.828\cdot 10^{-6}$ (R; Ref. 4), $4.408\cdot 10^{-6}$ (R; Ref. 6), $4.400\cdot 10^{-6}$ (R; Ref. 7), $4.2\cdot 10^{-6}$ (R; Ref. 9), $4.570\cdot 10^{-6}$ (R; Ref. 10), $1.76\cdot 10^{-6}$ (D; Ref. 11), $4.462\cdot 10^{-6}$ (R; Ref. 12), $4.453\cdot 10^{-6}$ (R; Ref. 13), $4.484\cdot 10^{-6}$ (R; Ref. 14), $5.6\cdot 10^{-6}$ (D; Ref. 15), $4.248\cdot 10^{-6}$ (R; Ref. 17), $4.210\cdot 10^{-6}$ (R; Ref. 18), $3.1\cdot 10^{-6}$ (T; Ref. 19), $4.231\cdot 10^{-6}$ (R; Ref. 20), $4.579\cdot 10^{-6}$ (R; Ref. 22), $4.639\cdot 10^{-6}$ (R; Ref. 23), $4.382\cdot 10^{-6}$ (R; Ref. 24)	$4.3\cdot 10^{-6}$
298.4	$4.317\cdot 10^{-6}$ (T; Ref. 3)	$4.4\cdot 10^{-6}$
299.5	$4.471\cdot 10^{-6}$ (T; Ref. 17)	$4.5\cdot 10^{-6}$
300.2	$4.799\cdot 10^{-6}$ (T; Ref. 14)	$4.6\cdot 10^{-6}$
302.4	$4.828\cdot 10^{-6}$ (T; Ref. 17)	$5.0\cdot 10^{-6}$
303.1	$5.241\cdot 10^{-6}$ (T; Ref. 24)	$5.2\cdot 10^{-6}$
303.5	$5.310\cdot 10^{-6}$ (T; Ref. 24)	$5.3\cdot 10^{-6}$
303.9	$5.632\cdot 10^{-6}$ (T; Ref. 3)	$5.3\cdot 10^{-6}$
305.0	$5.101\cdot 10^{-6}$ (T; Ref. 17)	$5.6\cdot 10^{-6}$
307.7	$6.231\cdot 10^{-6}$ (T; Ref. 24)	$6.2\cdot 10^{-6}$
308.3	$6.511\cdot 10^{-6}$ (T; Ref. 3)	$6.4\cdot 10^{-6}$
312.5	$7.702\cdot 10^{-6}$ (R; Ref. 3), $7.490\cdot 10^{-6}$ (R; Ref. 24)	$7.5\cdot 10^{-6}$
313.3	$7.733\cdot 10^{-6}$ (T; Ref. 24)	$7.8\cdot 10^{-6}$
317.9	$9.305\cdot 10^{-6}$ (T; Ref. 24)	$9.4\cdot 10^{-6}$
318.1	$9.684\cdot 10^{-6}$ (T; Ref. 3)	$9.5\cdot 10^{-6}$
323.2	$1.158\cdot 10^{-5}$ (T; Ref. 24)	$1.2\cdot 10^{-5}$
323.4	$1.168\cdot 10^{-5}$ (T; Ref. 24)	$1.2\cdot 10^{-5}$
328.8	$1.480\cdot 10^{-5}$ (T; Ref. 24)	$1.5\cdot 10^{-5}$
337.7	$2.190\cdot 10^{-5}$ (T; Ref. 24)	$2.3\cdot 10^{-5}$
346.6	$3.360\cdot 10^{-5}$ (T; Ref. 24)	$3.5\cdot 10^{-5}$
348.2	$3.629\cdot 10^{-5}$ (T; Ref. 24)	$3.7\cdot 10^{-5}$

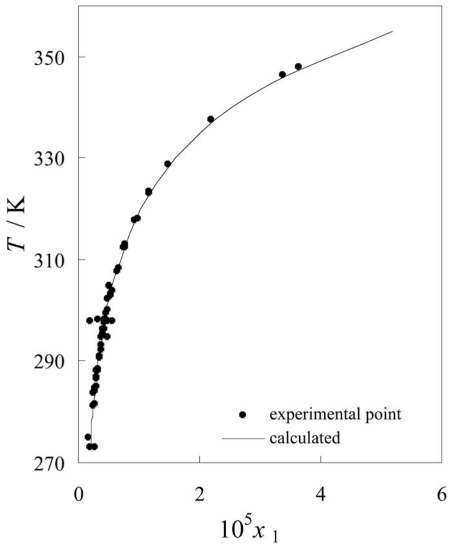

FIG. 1. All the solubility data for naphthalene (1) in water (2).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	M. Akiyoshi, T. Deguchi, and I. Sanemasa, Bull. Chem. Soc. Jpn. **60**, 3935 (1987).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(2.35 \pm 0.06) \cdot 10^{-4}$	$3.02 \cdot 10^{-3}$	$4.25 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Aqueous solutions saturated with vapor of (1) were prepared in the apparatus described in Sanemasa, *et al.*[1] Samples were extracted with $CHCl_3$, dehydrated, and (1) was determined with a Hitachi 100-50 spectrophotometer. Details of equilibrations and sampling were described in the paper. Measurements were repeated at least four times and average was taken as the solubility.

Source and Purity of Materials:

(1) Wako Pure and Nakarai Chemicals Co.; analytical grade, purity 98%; used as received.
(2) Distilled and de-ionized water.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: as above.

References:

[1] I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Values

The solubility of naphthalene in water at 25 °C was reported to be 0.00315 g (1)/100 g sln.

The corresponding mole fraction, x_1, value calculated by compiler is $4.42 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:

(1) Eastman Kodak Co. best grade; recrystallized from ethanol; melting point 80.5 °C.
(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	D. Bennett and W. J. Canady, J. Am. Chem. Soc. **106**, 910 (1984).
Variables:	**Prepared By:**
Temperature: 275.05–318.05 K	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

T/K	$10^3 \cdot g(1)/100$ g sln (compilers)	$10^6 \cdot x_1$
275.05	1.207	1.696
283.85	1.719	2.416
288.55	2.163	3.041
294.85	2.671	3.755
298.35	3.072	4.318
303.85	4.008	5.634
308.25	4.631	6.509
312.45	5.479	7.702
318.05	6.889	9.684

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. 0.2 g of naphthalene was added to 100 mL of water in a Virtis homogenizer flask, sealed, equilibrated for 30 min, and stirred at approximately 25 000 rpm for 2 min with Virtis Model 23 homogenizer. Details of equilibrations and sampling were given in Larese and Canady[1] and Larese *et al.*[2] The concentrations were determined with a Cary 17D spectrophotometer. Each experimental point is based on at least four measurements.

Source and Purity of Materials:

(1) Fisher Scientific Co.; zone refined and recrystallized from 95% ethanol; melting point 80–81 °C.
(2) Double-glass-distilled water.

Estimated Error:

Temperature: ±0.2 K.
Solubility: 1.8% (mean deviation).

References:

[1] R. J. Larese and W. J. Canady, J. Phys. Chem. **65**, 1240 (1961).
[2] R. J. Larese, D. A. Robinson, W. F. Brassine, and W. J. Canady, J. Phys. Chem. **66**, 897 (1962).

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).

Variables:

Temperature: 0–42.8 °C

Prepared By:

G. T. Hefter

Experimental Values

Solubility of naphthalene in water

$t/°C$	$10^6 \cdot x_1$	$10^3 \cdot g(1)/100\ g\ sln^a$ (compiler)
0.0	1.92	1.37
0.4	1.92	1.37
0.5	1.94	1.38
0.9	2.05	1.46
1.9	2.11	1.50
9.4	2.75	1.96
10.0	2.72	1.94
14.9	3.29	2.34
15.9	3.45	2.46
19.3	3.93	2.80
25.0	4.83^b	3.44^b
25.6	5.03	3.58
30.1	6.04	4.30
30.2	6.16	4.39
35.2	7.65	5.45
36.0	7.69	5.48
42.8	10.3	7.35

[a] Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer–Lambert law, the stated cell path length (1 cm), and the authors' "extinctioin coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g (1)/L sln which was then converted to g (1)/100 g sln by assuming a solution density of 1.00 kg/L.

[b] Given in the paper as 0.0344 g (1)/L sln.

Auxiliary Information

Method/Apparatus/Procedure:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24 h, and then allowed to settle for at least another 24 h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

Source and Purity of Materials:

(1) Allied Chemical & Dye Corp., purified by vacuum distillation.
(2) Air-free conductivity water, no other details given.

Estimated Error:

Temperature: ±0.02 °C.
Solubility: ±0.5% relative.

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. T. Coyle, T. C. Harmon, and I. H. Suffet, Environ. Sci. Technol. **31**, 384 (1997).

Variables:

One temperature: 22 °C

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

$t/°C$	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
22	33.9	$3.39 \cdot 10^{-3}$	$4.77 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The generator column technique was used. The dynamic coupled column liquid chromatography method, described in May *et al.*,[1] was based on generating saturated solutions by pumping water through a column packed with glass beads that were previously coated with component (1). The concentration of (1) in the effluent of the generator column was measured by standard hplc techniques with an ultraviolet (UV) detector (Hewlett Packard Model 1050). The mean of three measurements is reported.

Source and Purity of Materials:

(1) Sigma Chemicals; purity 98%; used as received.
(2) Not specified.

Estimated Error:

Temperature: ±1 °C.
Solubility: 4.9% (relative standard deviation).

References:

[1] W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	R. M. Dickhut, A. W. Andren, and D. E. Armstrong, J. Chem. Eng. Data **34**, 438 (1989).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility naphthalene in water

t/°C	mg (1)/L sln	$10^4 \cdot$ g (1)/100 g sln (compilers)	$10^6 \cdot x_1$ (compilers)
25.0	29.1	2.92	4.11^a
	31.3±0.36	3.14	4.41^b
	31.3±0.62	3.14	4.41^b

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Saturated solutions were prepared by adding an excess of (1) to a glass bottle containing (2). The contents was mixed at room temperature for 24 h[a] or 36 h[b] on magnetic stirrer and equilibrated for additional 24 h[a] or 36 h[b] in a water bath. Samples were filtered and absorbance in 50/50 aqueous methanol was measured at 254 nm by use of a Varian UV spectrophotometer and by hplc. Each replicate was sampled and analyzed two or three times. Reported solubility was the average of 35[a] and 3[b] replicates.

Source and Purity of Materials:

(1) Source not specified; scintillation grade; purity 99%; used as received.
(2) Distilled, purified by Milli-Q system, UV oxidized for 3 h prior to use.

Estimated Error:

Temperature: ±0.5 K.
Solubility: Standard deviation as above.

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of naphthalene in water at 25 °C was reported to be 31.3 mg (1)/kg (2) and $2.43 \cdot 10^{-4}$ mol(1)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $3.13 \cdot 10^{-3}$ g (1)/100 g sln and $4.40 \cdot 10^{-6}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen, and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors (FIDS) was employed.

Source and Purity of Materials:

(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Double distilled; free of trace organics.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: ±0.4 mg (1)/kg (2) (from 8 determinations).

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	J. E. Gordon and R. L. Thorne, J. Phys. Chem. **71**, 4390 (1967).
Variables:	**Prepared By:**
One temperature: 24.91 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
24.91	$(2.611\pm0.015)\cdot10^{-4}$	$3.356\cdot10^{-3}$	$4.718\cdot10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

An excess of naphthalene and 15 mL of water were sealed in 20 mm diam Pyrex ampoules. These were rocked in a constant temperature bath. Samples were equilibrated for at least 24 h and next filtered. Details of filtration were described in the paper. Concentrations were calculated from the optical densities (absorbances) measured by a Cary Model 14 spectrophotometer. The reported value is a mean of 11 determinations at various equilibration times, each an average of measurements at 3 wavelengths.

Source and Purity of Materials:

(1) Distillation Products Industries, White Label Material; recrystallized four times from ethanol and sublimated; or James Hinton, Valpariso, Fla.; zone-refined material, purity>99.99%.
(2) Laboratory distilled water, de-ionized, distilled from $KMnO_4$, and redistilled.

Estimated Error:
Temperature: ±0.03 °C.
Solubility: As above.

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	S. Hilpert, Angew. Chem. **29**, 57 (1916).
Variables:	**Prepared By:**
Temperature: 0 and 25 °C	A. Maczynski and A. Szafranski

Experimental Values

Solubility of naphthalene in water

t/°C	$10^6\cdot x_1$	$10^3\cdot$ g (1)/100 g sln
0	2.7	1.9
25	4.2	3.0

Auxiliary Information

Method/Apparatus/Procedure:

A sample of (1) was shaken with 1000 g (2) until saturation and then filtered. The filtrate was steam distilled to drive away (1) which was collected and presumably weighed.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. Janado, Y. Yano, Y. Doi, and H. Sakamoto, J. Solution Chem. **12**, 741 (1983).

Variables:

One temperature: 25.0 °C

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

$t/°C$	mg (1)/L (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	32.4	$3.25 \cdot 10^{-3}$	$4.57 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. About 10 g of water with an excess of naphthalene was placed in a thermostat, stirred for 6 h, gently shaken for another 18 h, and allowed to stand for separation for the next 6 h. A portion of a clear solution was placed in a 15 mL vial containing a weighted amount of *n*-hexane. After extracting into *n*-hexane, naphthalene was determined by spectrophotometry.

Source and Purity of Materials:

(1) Nakarai Chemicals Ltd.; analytical grade; used as received.
(2) Glass redistilled water.

Estimated Error:

Temperature: ±0.05 °C.
Solubility: <1.0% (average deviation from the mean).

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of naphthalene in water at 25 °C was reported to be 0.0125 g (1)/L sln and $9.75 \cdot 10^{-5}$ mol(1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln, the corresponding values calculated by the compiler are 0.00125 g (1)/100 g sln and mole fraction, $x_1 = 1.76 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of naphthalene in water at 25 °C was reported to be 31.7 mg (1)/L sln and $x_1 = 4.46 \cdot 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00317 g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:

Solubility: ±0.26 mg(1)/L sln (max. dev. from several determinations).

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of naphthalene in water at 25 °C was reported to be 31.69 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, values calculated by compiler are 0.003169 g (1)/100 g sln and $4.425 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

The dynamic coupled column liquid chromatography (dcclc) method was based on generating saturated solutions by pumping water through a column packed with glass beads that had been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:

(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

Estimated Error:

Temperature: ±0.05 °C.
Solubility: ±0.23 mg (1)/100 kg (2) (standard deviation)

References:

[1] W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. E. May, S. P. Wasik, M. M. Miller, Y. B. Tewari, J. M. Brown-Thomas, and R. N. Goldberg, J. Chem. Eng. Data **28**, 197 (1983).

Variables:

Temperatures: 281.35–300.15 K

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

T/K	$10^3 \cdot$ g (1)/100 g sln (compilers)	$10^6 \cdot x_1$
281.35	1.6904	2.376
284.65	1.9230	2.703
286.55	2.0368	2.863
288.25	2.1478	3.019
292.45	2.5782	3.624
296.55	2.9467	4.142
298.15	3.1907	4.485
300.15	3.4141	4.799

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were determined by an automated coupled-column liquid chromatographic apparatus; technique and apparatus were reported in May *et al.*[1] and Tewarti *et al.*[2] A saturated solution was generated by pumping water through a column containing the solute coated on Chromosorb W. The hplc method and UV detection were used for analysis.

Source and Purity of Materials:

(1) Source not specified; purity>99 mole % by glc.
(2) Not specified.

Estimated Error:

Temperature: ±0.1 K (Tewari *et al.*[2]).

References:

[1] W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

[2] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

S. Mitchell, J. Chem. Soc. 1332 (1926).

Variables:

Temperature: 15 and 25 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

Solubility of naphthalene in water

t/°C	$10^6 \cdot x_1$ (compiler)	g (1)/100 g sln (compiler)	g (1)/L sln (2)
15	3.1	0.0022	0.022
25	5.6	0.0040	0.040

Auxiliary Information

Method/Apparatus/Procedure:

For this study an interferometer of the type described in Jamin,[1] was constructed.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

References:

[1] Jamin, Ann. Chim. Phys. **52**, 171 (1958).

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

S. Sawamura, M. Tsuchiya, T. Ishigami, Y. Taniguchi, and K. Suzuki, J. Solution Chem. **22**, 727 (1993).

Variables:

Temperature: 25.00 °C
Pressure: 45.4–207.3 MPa

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

$t/°C$	P/MPa	$10^3 \cdot$ g (1)/100 g sln (compilers)	$10^6 \cdot x_1$
25.00	45.4	2.40	3.38
	69.1	2.11	2.97
	98.7	1.76	2.48
	148.1	1.39	1.95
	156.0	1.24	1.74
	207.3	0.953	1.34

Auxiliary Information

Method/Apparatus/Procedure:

The pressure vessel for preparation of a saturated solution at high pressure, and the method used to measure the solubilities were described in Sawamura *et al.*[1] Pressure was monitored with a gauge of Bourdon-tube type (Heise, fullscale 400 MPa and 0.5 MPa divisions). Temperature of the water bath was measured by a platinum resistance thermometer. Samples were taken after shaking for at least 40 h and filtration under high pressure. The concentration of (2) in (1) was determined on the basis of measurements of the ultraviolet absorption spectrum (Hitachi Model 139 spectrophotometer) and recommended solubility values at 25.00 °C and 0.1 MPa reported in Shaw.[2]

Source and Purity of Materials:

(1) Nakarai Tesque; recrystallized four times from ethanol and sublimed.
(2) Distilled after de-ionization.

Estimated Error:

Temperature: ±0.05 °C.

References:

[1] S. Sawamura, S. Yasyhara, N. Sugi, and N. Egoshi, Bull. Soc. Chem, Jpn. **66**, 2406 (1993).

[2] D. G. Shaw, ed., *IUPAC Solubility Data Series*, Vol. 38 (Pergamon, New York, 1989).

Components:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).

Variables:

One temperature: 25.0 °C

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

$t/°C$	μg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$2.2 \cdot 10^4$	$2.2 \cdot 10^{-3}$	$3.1 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was calculated from fluorescence measurements. A saturated solution was prepared by slowly stirring an excess of hydrocarbon in water for several days in a sealed flask. The sample was then diluted over 2 orders of magnitude by the addition of known volumes of water. Details of sample preparation, apparatus, and measurements were described in the paper.

Source and Purity of Materials:

(1) Source not specified; recrystallized from a solvent.
(2) Distilled and passed through a Sephadex column.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz and S. P. Wasik, J. Chem. Eng. Data **22**, 270 (1977).
Variables:	**Prepared By:**
Temperature: 12–25 °C	A. Maczynski

Experimental Values

Solubility of naphthalene in water

$t/°C$	$10^6 \cdot x_1$ (compiler)	$10^3 \cdot$ g (1)/100 g sln (compiler)	$10^4 \cdot$ mol(1)/L
12	2.83	2.01	1.57
18	3.42	2.43	1.90
25	4.21	3.00	2.34

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) is too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.

Source and Purity of Materials:

(1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole %.
(2) Distilled from $KMnO_4$ and passed through a Sephadex column.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: $\pm 2.10^{-6}$ mol (1)/L.

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
Variables:	**Prepared By:**
Temperature: 8.4–31.8 °C	A. Maczynski

Experimental Values

Solubility of naphthalene in water

$t/°C$	$10^6 \cdot x_1$ (compiler)	$10^3 \cdot$ g (1)/100 g sln (compiler)	$10^4 \cdot$ mol (1)/L
8.4	2.52	1.79	1.40±0.02
11.1	2.68	1.91	1.49±0.03
14.0	2.99	2.13	1.66±0.05
17.5	3.39	2.41	1.88±0.03
20.2	3.73	2.65	2.07±0.02
23.2	4.00	2.85	2.22±0.03
25.0	4.25	3.03	2.36±0.02
26.3	4.47	3.18	2.48±0.02
29.2	4.83	3.44	2.68±0.02
31.8	5.10	3.63	2.83±0.02

Auxiliary Information

Method/Apparatus/Procedure:

Two methods were used. At 25 °C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry, and placed in the fluorimeter.

Source and Purity of Materials:

(1) Source not specified; better than 99.9 mole %, by glc; used as received.
(2) Distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: see above.

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

T/K	mol (1)/g (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
298.15	$(2.51\pm0.02)\cdot10^{-7}$	$3.22\cdot10^{-5}$	$4.52\cdot10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The radiometric method was used. The equilibration was carried out in a modified vessel,[1] equipped with a magnetic stirrer. The temperature of the water bath was maintained within ±0.05 K. Equilibrium was obtained after several days and then samples were filtered through a glass wool plug. Analyses were performed by counting the radioactivity on an LKB–Wallac 81000 liquid scintillation counter. At least 5 parallel determinations were performed.

Source and Purity of Materials:

(1) Mixture of $[1\text{-}^{14}C]$naphthalene from the Radiochemical Center, specific activity 200 mCi/mmol and radiochemical purity 99%, with inactive naphthalene; Recrystallized from ethanol.
(2) Distilled water passed through an Amberlite CG 120 +CG 400 ion-exchange column.

Estimated Error:
Temperature: ±0.05 K.
Solubility: As above.

References:
[1] F. Franks, M. Gent, and H. H. Johnson, J. Chem. Soc. 2716 (1963).

Components:
(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Vesala and H. Lönnberg, Acta Chem. Scand., Ser. A **34**, 187 (1980).

Variables:
One temperature: 298.2 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

T/K	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
298.2	$(2.54\pm0.006)\cdot10^{-4}$	$3.26\cdot10^{-3}$	$4.58\cdot10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The radiometric method was used. The equilibration was carried out in the stoppered Sovirel tubes, with a volume of about 10 mL, by periodic shaking for 1 week in a thermostated water bath. Samples were taken by a Finnpipette through a glass wool plug. Analyses were performed by counting the radioactivity on an LKB–Wallac 81000 liquid scintillation counter. The reported value is the mean from six determinations.

Source and Purity of Materials:

(1) Mixture of $[1\text{-}^{14}C]$naphthalene from the Radiochemical Center, specific activity 7400 MBq/mmol, with inactive naphthalene from BDH, analytical reagent; recrystallyzed from ethanol.
(2) Not stated.

Estimated Error:
Not stated.

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).
Variables:	**Prepared By:**
Temperature: 0–75 °C	A. Maczynski

Experimental Values

Solubility of naphthalene in water

t/°C	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2) experiment	mg (1)/kg (2) smoothed with (standard deviation)
0.0	—			13.7 (0.2)
22.2	3.98	0.00283	28.8, 29.1, 28.8	28.3
24.5	4.31	0.00307	30.8 (2), 30.1 (2), 30.7	30.7
25.0	4.38	0.00312		31.2 (0.2)
29.9	5.24	0.00373	38.1, 38.2, 38.3	37.3
30.3	5.31	0.00378	38.1, 37.6, 37.6	37.8
34.5	6.23	0.00443	44.6, 43.8	44.3
39.2	7.49	0.00533	52.6, 52.8	53.3
40.1	7.73	0.00550	54.8	55.0
44.7	9.30	0.00662	66.0, 65.5, 65.3	66.2
50.0	11.58	0.00824		82.4 (0.4)
50.2	11.68	0.00831	78.6	83.1
55.6	14.8	0.0105	106	105
64.5	21.9	0.0156	166, 151, 157	156
73.4	33.6	0.0239	240, 247, 244	239
75.0	36.3	0.0258		258 (3)

Auxiliary Information

Method/Apparatus/Procedure:

Approximately 20 g of (1) was placed in each of three 250 mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from 1 to 3 weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1–0.2 g of samples followed by serial dilution in calibrated glassware.

Source and Purity of Materials:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.
(2) Distilled and de-ionized.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: See experimental values above.

Components:	**Original Measurements:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	F. M. Van Meter and H. M. Neumann, J. Am. Chem. Soc. **98**, 1382 (1976).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of naphthalene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1
25.0	$2.34 \cdot 10^{-4}$	$3.01 \cdot 10^{-3}$	$4.23 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A 100 mL volumetric flask of water and 1.0 g of naphthalene flakes were thermostatted in an aquarium bath at 25±0.1 °C and agitated continuously. Quantities of this solution were filtered and the absorbance was measured in 5.00 cm matched silica cells on a Cary 14 spectrophotometer. Three solubility measurements were made.

Source and Purity of Materials:

(1) Source not specified; recrystallized from methanol; melting point 80.0 °C.
(2) Distilled water.

Estimated Error:

Temperature: ±0.1 °C.

2.2. 1,2,3,4-Tetrahydronaphthalene+Water

Components:	**Evaluators:**
(1) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of 1,2,3,4-Tetrahydronaphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Economou *et al.*[1] at 374–596 K and 112–13 162 kPa, and Christensen and Paulaitis[2] at 573 K and 9758 kPa.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1=\ln x_{1,\min}+D[(T_{\min}/T)\ln(T_{\min}/T)+1-(T_{\min}/T)], \qquad (1)$$

where: $\ln x_{1,\min}=-11.50$; $D=45.68$; $T_{\min}=290$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 3. The data of Christensen and Paulaitis[2] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. All the remaining data are in are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in 1,2,3,4-Tetrahydronaphthalene (1)

The experimental solubility data for (2) in (1) have been investigated by Economou *et al.*[1] at 374–596 K and 112–13 162 kPa, and Christensen and Paulaitis[2] at 573 K and 9889 kPa.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2=d_1+d_2(1/T_r-1)+d_3(1-T_r)^{1/3}+d_4(1-T_r), \qquad (2)$$

where: $d_1=-0.067$; $d_2=-0.330$; $d_3=1.477$; $d_4=-13.343$; $T_r=T/615.1$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1,2,3,4-tetrahydronaphthalene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 4 and shown in Fig. 2. The data of Economou *et al.*[1] at 424–596 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Christensen and Paulaitis,[2] and Economou *et al.*[1] at 324 K are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

High Pressure Solubility of 1,2,3,4-Tetrahydronaphthalene (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by Christensen and Paulaitis[2] at 573 K and 10 447–16 303 kPa, have not been critically evaluated because the developed method is not applied for such data.

Rejected and Inaccessible Data

The data reported by Jockers *et al.*[3] at 597–663 K and 12 500–132 000 kPa lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1] I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

[2] S. P. Christensen and M. E. Paulaitis, Fluid Phase Equilib. **71**, 63 (1992).

[3] R. Jockers, R. Paas, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **81**, 1093 (1977).

TABLE 3. Experimental values for solubility of 1,2,3,4-tetrahydronaphthalene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
374.2	112.4 (Ref. 1)	$9.20\cdot 10^{-6}$ (D; Ref. 1)	$3.5\cdot 10^{-5}$
424.7	506.8 (Ref. 1)	$1.71\cdot 10^{-5}$ (D; Ref. 1)	$1.3\cdot 10^{-4}$
475.2	1689 (Ref. 1)	$3.60\cdot 10^{-5}$ (D; Ref. 1)	$5.7\cdot 10^{-4}$
573.2	9758 (Ref. 2)	$9.00\cdot 10^{-3}$ (T; Ref. 2)	$9.3\cdot 10^{-3}$
576.2	9942 (Ref. 1)	$1.66\cdot 10^{-4}$ (D; Ref. 1)	$1.0\cdot 10^{-2}$
595.9	13 162 (Ref. 1)	$6.10\cdot 10^{-2}$ (D; Ref. 1)	$1.7\cdot 10^{-2}$

TABLE 4. Experimental values for solubility of water (2) in 1,2,3,4-tetrahydronaphthalene (1)

T/K	P/kPa	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
374.2	112.4 (Ref. 1)	$2.06\cdot 10^{-2}$ (D; Ref. 1)	$1.2\cdot 10^{-2}$
424.7	506.8 (Ref. 1)	$4.40\cdot 10^{-2}$ (T; Ref. 1)	$3.5\cdot 10^{-2}$
475.2	1689 (Ref. 1)	$1.20\cdot 10^{-1}$ (T; Ref. 1)	$1.0\cdot 10^{-1}$
573.2	9889 (Ref. 2)	$4.28\cdot 10^{-1}$ (D; Ref. 2)	$6.7\cdot 10^{-1}$
576.2	9942 (Ref. 1)	$5.47\cdot 10^{-1}$ (T; Ref. 1)	$7.1\cdot 10^{-1}$
595.9	13 162 (Ref. 1)	$9.39\cdot 10^{-1}$ (T; Ref. 1)	$9.7\cdot 10^{-1}$

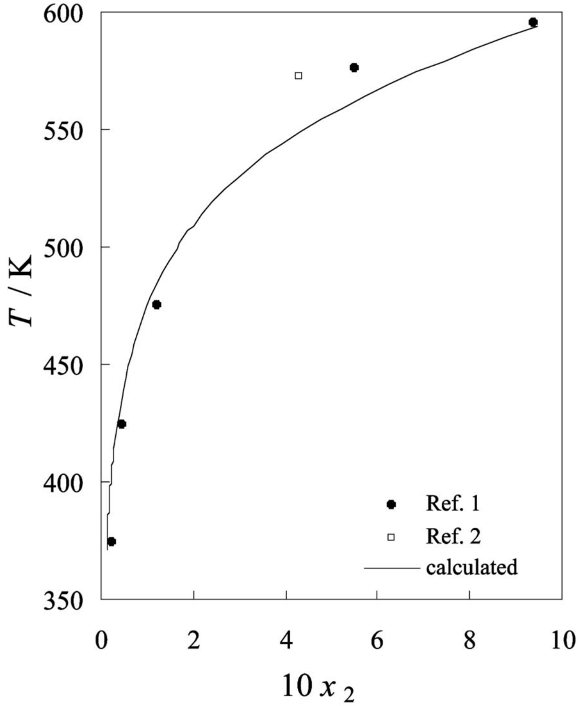

FIG. 2. All the solubility data for water (2) in 1,2,3,4-tetrahydronaphthalene (1).

Components:

(1) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

S. P. Christensen and M. E. Paulaitis, Fluid Phase Equilib. **71**, 63 (1992).

Variables:

One temperature: 300.0 °C
Pressure: 94.3–160.9 atm

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Mutual solubility of 1,2,3,4-tetrahydronaphthalene and water

t/°C	P/atm	g (1)/100 g sln (compilers)	x_1
300.0	94.3[a]	—	—
	96.3	6.2	0.009
	96.9	6.9	0.010
	97.6	4.2	0.006
	107.5	5.6	0.008
	111.2	5.6	0.008
	121.4	4.2	0.006
	121.4	5.6	0.008
	121.4	4.9	0.007
	134.0	5.6	0.008
	134.0	4.9	0.007
	160.5	4.9	0.007
	160.9	4.9	0.007

Mutual solubility of water in 1,2,3,4-tetrahydronaphthalene

t/°C	P/atm	g (2)/100 g sln (compilers)	x_2
300.0	97.6	15.4	0.572
	103.1	15.5	0.574
	107.5	15.0	0.565
	121.4	14.4	0.552
	121.4	14.6	0.556
	121.4	14.5	0.555
	134.0	13.9	0.543
	160.5	13.1	0.525
	160.9	13.1	0.525

[a] Three phase pressure.

Auxiliary Information

Method/Apparatus/Procedure:

A flow technique was used. The apparatus contained a high-pressure view cell (60 mL volume), was equipped with sapphire windows, and was placed in a nitrogen bath.[1] The system pressure was measured to within ±0.1 atm with a Heise bourdon-tube gauge (Gregory Model CM). The temperature was measured with platinum resistance thermometer (Burns Engineering Co.) to within ±0.1 °C. Equilibrium phase compositions were measured with a Perkin-Elmer gas chromatograph (Model 3920 B) equipped with a Porapak P column and a thermal conductivity detector.

Source and Purity of Materials:

(1) Aldrich; purity 99%; used as received.
(2) Distilled and de-ionized.

Estimated Error:

Temperature: ±0.1 °C.
Pressure: ±0.1 atm.

References:

[1] M. C. Thies and M. E. Paulaitis, J. Chem. Eng. Data **29**, 438 (1984).

Components:

(1) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Variables:

Temperature: 374.15–595.92 K
Pressure: 0.1124–13.162 MPa

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1,2,3,4-tetrahydronaphthalene in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^2 \cdot x_1$
374.15	0.1124	0.006751	0.000920
424.65	0.5068	0.01255	0.00171
475.15	1.689	0.02641	0.00360
576.15	9.942	0.1217	0.0166
595.92[a]	13.162	32.28	6.1

Solubility of water in 1,2,3,4-tetrahydronaphthalene

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
374.15	0.1124	0.286	0.0206
424.65	0.5068	0.623	0.0440
475.15	1.689	1.82	0.120
576.15	9.942	14.13	0.547
595.92[a]	13.162	67.72	0.939

[a] Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of (1) in (2) was measured by glc, while that of (2) in (1) by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus.

Source and Purity of Materials:

(1) Aldrich; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:

Temperature: ±0.6 K at critical end point.[a]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[a]
Pressure: 1% and ±0.04 MPa at critical end point.[a]

References:

[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

Components:	Original Measurements:
(1) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2] (2) Water; H_2O; [7732-18-5]	R. Jockers, R. Paas, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **81**, 1093 (1977).
Variables:	**Prepared By:**
Temperature: 324.0–390.0 °C Pressure: 125–1320 bar	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Critical data of 1,2,3,4-tetrahydronaphthalene and water

$t/°C$	P/bar
324.0[a]	125
330.0	200
340.0	332
350.0	462
360.0	645
370.0	835
380.0	1055
390.0	1320

[a] Critical end point of three-phase (liquid–liquid-gas) line.

Auxiliary Information

Method/Apparatus/Procedure:

The measurements on 1,2,3,4-tetrahydronaphthalene–water mixtures were made in an optical high temperature high pressure autoclave with magnetic stirring described in Alwani and Schneider.[1] No more details were reported in the paper.

Source and Purity of Materials:

(1) Not stated
(2) Not stated.

Estimated Error:

Not stated.

References:

[1] Z. Alwani and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **73**, 294 (1969).

2.3. Butylbenzene+Water

Components:	Evaluators:
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of Butylbenzene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Andrews and Keefer[1]	298	Massaldi and King[7]	298
Chen and Wagner[2]	303–373 (136–238 kPa)	Owens *et al.*[8]	280–318
Dohanyosova *et al.*[3]	273–318	Sutton and Calder[9]	298
Klevens[6]	298	Tewari *et al.*[10]	298

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \qquad (1)$$

where $\ln x_{1,\min} = -12.98$; $D = 51.95$; and $T_{\min} - 290$ K.

Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 5.

All the experimental and reference data are listed in Table 6 and shown in Fig. 3.

Critical Evaluation of the Solubility of Water (2) in Butylbenzene (1)

The experimental solubility data for (2) in (1) have been investigated by Chen and Wagner[2] at 303–373 K, Englin *et al.*[4] at 283–303 K, and Jones and Monk[5] at 298–308 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \qquad (2)$$

where: $d_1 = -0.232$; $d_2 = -2.326$; $d_3 = 0.400$; $d_4 = -7.774$; and $T_r = T/588.0$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of butylbenzene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 7 and shown in Fig. 4. The data of Jones and Monk[5] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful. The data of Chen and Wagner,[2] and Englin *et al.*[4] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:

[1] L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[2] H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).
[3] P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001).
[4] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[5] J. R. Jones and C. B. Monk, J. Chem. Soc. 2633 (1963).
[6] H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[7] H. A. Massaldi and C. J. King, J. Chem. Eng. Data **18**, 393 (1973).
[8] J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).
[9] C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[10] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

TABLE 5. The data categories for solubility of butylbenzene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
273.7			Dohanyosova *et al.*[3]
278.2			Dohanyosova *et al.*[3]
280.2		Owens *et al.*[8]	
283.2		Owens *et al.*[8]	
285.7		Owens *et al.*[8]	
288.2		Owens *et al.*[8]	Dohanyosova *et al.*[3]
290.7		Owens *et al.*[8]	
293.2		Owens *et al.*[8]	
298.2	Massaldi and King,[7] Owens *et al.*,[8] Tewari *et al.*[10]	Dohanyosova *et al.*[3]	Andrews and Keefer,[1] Klevens,[6] Sutton and Calder[9]
303.2	Chen and Wagner,[2] Owens *et al.*[8]		
308.2	Dohanyosova *et al.*,[3] Owens *et al.*[8]		
313.2	Chen and Wagner,[2] Owens *et al.*[8]		
318.2	Dohanyosova *et al.*,[3] Owens *et al.*[8]		
323.2		Chen and Wagner[2]	
328.2		Chen and Wagner[2]	
333.2		Chen and Wagner[2]	
343.2		Chen and Wagner[2]	
353.2		Chen and Wagner[2]	
363.2		Chen and Wagner[2]	
373.2		Chen and Wagner[2]	

TABLE 6. Experimental values for solubility of butylbenzene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.7		$1.55\cdot 10^{-6}$ (D; Ref. 3)	$2.5\cdot 10^{-6}$
278.2		$1.54\cdot 10^{-6}$ (D; Ref. 3)	$2.4\cdot 10^{-6}$
280.2		$1.79\cdot 10^{-6}$ (T; Ref. 8)	$2.4\cdot 10^{-6}$
283.2		$1.74\cdot 10^{-6}$ (T; Ref. 8)	$2.3\cdot 10^{-6}$
285.7		$1.77\cdot 10^{-6}$ (T; Ref. 8)	$2.3\cdot 10^{-6}$
288.2		$1.52\cdot 10^{-6}$ (D; Ref. 3), $1.74\cdot 10^{-6}$ (T; Ref. 8)	$2.3\cdot 10^{-6}$
290.7		$1.77\cdot 10^{-6}$ (T; Ref. 8)	$2.3\cdot 10^{-6}$
293.2		$1.84\cdot 10^{-6}$ (T; Ref. 8)	$2.3\cdot 10^{-6}$
298.2		$1.69\cdot 10^{-7}$ (D; Ref. 1), $1.65\cdot 10^{-6}$ (T; Ref. 3), $6.70\cdot 10^{-6}$ (D; Ref. 6), $2.40\cdot 10^{-6}$ (R; Ref. 7), $1.85\cdot 10^{-6}$ (R; Ref. 8), $1.58\cdot 10^{-6}$ (D; Ref. 9), $1.86\cdot 10^{-6}$ (R; Ref. 10)	$2.4\cdot 10^{-6}$
303.2	136 (Ref. 2)	$2.24\cdot 10^{-6}$ (R; Ref. 2), $1.96\cdot 10^{-6}$ (R; Ref. 8)	$2.4\cdot 10^{-6}$
308.2		$1.95\cdot 10^{-6}$ (R; Ref. 3), $2.08\cdot 10^{-6}$ (R; Ref. 8)	$2.5\cdot 10^{-6}$
313.2	136 (Ref. 2)	$2.39\cdot 10^{-6}$ (R; Ref. 2), $2.24\cdot 10^{-6}$ (R; Ref. 8)	$2.7\cdot 10^{-6}$
318.2		$2.39\cdot 10^{-6}$ (R; Ref. 3), $2.57\cdot 10^{-6}$ (R; Ref. 8)	$2.8\cdot 10^{-6}$
323.2	136 (Ref. 2)	$2.73\cdot 10^{-6}$ (T; Ref. 2)	$3.1\cdot 10^{-6}$
328.2		$2.86\cdot 10^{-6}$ (T; Ref. 3)	$3.3\cdot 10^{-6}$
333.2	136 (Ref. 2)	$3.61\cdot 10^{-6}$ (T; Ref. 2)	$3.6\cdot 10^{-6}$
343.2	136 (Ref. 2)	$4.30\cdot 10^{-6}$ (T; Ref. 2)	$4.5\cdot 10^{-6}$
353.2	136 (Ref. 2)	$6.40\cdot 10^{-6}$ (T; Ref. 2)	$5.6\cdot 10^{-6}$
363.2	204 (Ref. 2)	$8.20\cdot 10^{-6}$ (T; Ref. 2)	$7.2\cdot 10^{-6}$
373.2	238 (Ref. 2)	$1.12\cdot 10^{-5}$ (T; Ref. 2)	$9.3\cdot 10^{-6}$

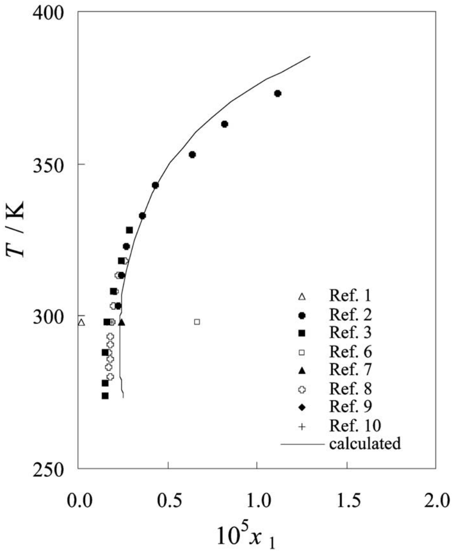

FIG. 3. All the solubility data for butylbenzene (1) in water (2).

TABLE 7. Experimental values for solubility of water (2) in butylbenzene (1)

T/K	P/kPa	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
283.2		$1.74\cdot 10^{-3}$ (T; Ref. 4)	$1.6\cdot 10^{-3}$
293.2		$2.46\cdot 10^{-3}$ (T; Ref. 4)	$2.1\cdot 10^{-3}$
298.2		$3.50\cdot 10^{-4}$ (D; Ref. 5)	$2.5\cdot 10^{-3}$
303.2	136 (Ref. 2)	$2.36\cdot 10^{-3}$ (T; Ref. 2), $3.33\cdot 10^{-3}$ (T; Ref. 4), $4.1\cdot 10^{-4}$ (D; Ref. 5)	$2.8\cdot 10^{-3}$
308.2		$4.9\cdot 10^{-4}$ (D; Ref. 5)	$3.2\cdot 10^{-3}$
313.2	136 (Ref. 2)	$3.15\cdot 10^{-3}$ (T; Ref. 2)	$3.7\cdot 10^{-3}$
323.2	136 (Ref. 2)	$4.13\cdot 10^{-3}$ (T; Ref. 2)	$4.8\cdot 10^{-3}$
333.2	136 (Ref. 2)	$5.95\cdot 10^{-3}$ (T; Ref. 2)	$6.2\cdot 10^{-3}$
343.2	136 (Ref. 2)	$8.37\cdot 10^{-3}$ (T; Ref. 2)	$8.0\cdot 10^{-3}$
353.2	136 (Ref. 2)	$1.07\cdot 10^{-2}$ (T; Ref. 2)	$1.0\cdot 10^{-2}$
363.2	204 (Ref. 2)	$1.48\cdot 10^{-2}$ (T; Ref. 2)	$1.3\cdot 10^{-2}$
373.2	238 (Ref. 2)	$1.99\cdot 10^{-2}$ (T; Ref. 2)	$1.6\cdot 10^{-2}$

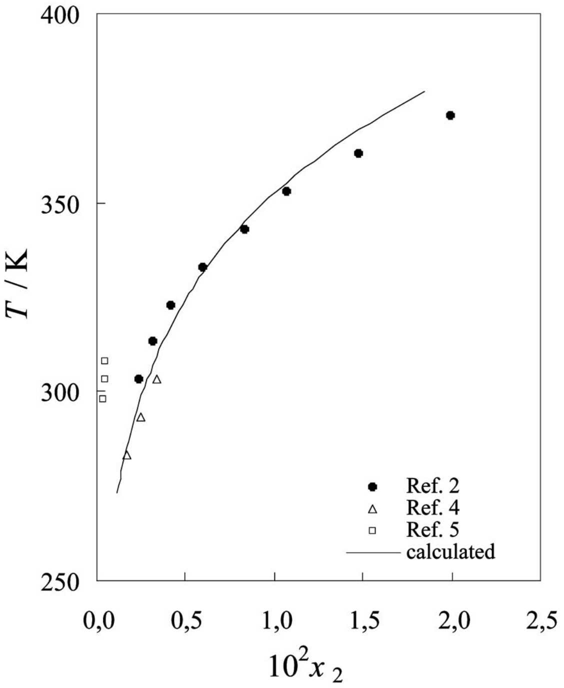

FIG. 4. All the solubility data for water (2) in butylbenzene (1).

Components:	**Original Measurements:**
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Values

The solubility of butylbenzene in water at 25 °C was reported to be 0.000126 g (1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $1.69\cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:

(1) Eastman Kodak Co. best grade; fractionally distilled; boiling point range 182.0–183.0 °C.

(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).

Variables:	**Prepared By:**
Temperature: 303.15–373.15 K Pressure: 1.36–2.38 bar	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of butylbenzene in water

T/K	P/bar	g (1)/100 g sln (compilers)	$10^6 \cdot x_1$
303.15	1.36	0.00167	0.224±0.012
313.15	1.36	0.00178	0.239±0.017
323.15	1.36	0.00203	0.273±0.010
333.15	1.36	0.00269	0.361±0.010
343.15	1.36	0.00320	0.430±0.011
353.15	1.36	0.00477	0.640±0.020
363.15	2.04	0.00611	0.820±0.043
373.15	2.38	0.00834	1.12±0.01

Solubility of water in butylbenzene

T/K	P/bar	g (2)/100 g sln (compilers)	$10^2 \cdot x_2$
303.15	1.36	0.0317	0.236±0.010
313.15	1.36	0.0424	0.315±0.006
323.15	1.36	0.0556	0.413±0.007
333.15	1.36	0.0803	0.595±0.027
343.15	1.36	0.1132	0.837±0.033
353.15	1.36	0.1450	1.07±0.05
363.15	2.04	0.2012	1.48±0.03
373.15	2.38	0.2718	1.99±0.08

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The continuous flow equilibrium apparatus for mutual solubility measurements[1] was used. Samples were collected in 25 mL vials and 60 and 120 mL bottles containing anhydrous ethanol or dichloromethane as solvent. Details of the standard preparation, calibration, and sampling procedures were described in Chen and Wagner.[2] A Hewlett-Packard 5880A gas chromatograph equipped with Porapac Q or GlasChrom 254 columns and a thermal conductivity detector was used for analysis. Reported solubilities are the average of 3–6 replicate determinations.

Source and Purity of Materials:

(1) Aldrich Chemical Co.; purity >99 mole %; used as received.
(2) Distilled and de-ionized water.

Estimated Error:

Temperature: ±0.2 K.
Solubility: standard deviation as above.

References:

[1] H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 470 (1994).
[2] H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 475 (1994).

Components:	**Original Measurements:**
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001).

Variables:	**Prepared By:**
Temperature: 273.65–328.15 K	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of butylbenzene in water

T/K	$10^4 \cdot$ mol (1)/L sln	$10^3 \cdot$ g (1)/100 g sln (compilers)	$10^6 \cdot x_1$
273.65	0.860	1.15	1.55
278.15	0.855	1.15	1.54
288.15	0.843	1.13	1.52
298.15	0.913	1.23	1.65
308.25	1.08	1.45	1.95
318.15	1.31	1.78	2.39
328.15	1.56	2.13	2.86

Auxiliary Information

Method/Apparatus/Procedure:

The solute vapor absorption method for preparation of the saturated solutions was used. Details of the apparatus, saturation procedure, and sampling are described in the paper. The temperature was measured with calibrated standard mercury thermometer to ±0.01 K. The samples were analyzed using a high performance liquid chromatograph (Ecom, Prague, Czech Republic) equipped with a Model LCP 4100 hplc pump, a Model LCD 2082 UV detector, and a C18 glass analytical column. The analysis of each sample was replicated 6–10 times.

Source and Purity of Materials:

(1) Aldrich Chemical Co.; purity >99%, confirmed by liquid and gas chromatography, used as received.
(2) Distilled and treated by a Milli-Q water purification system.

Estimated Error:

Temperature: ±0.01 K.

Components:
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 10–30 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in butylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	1.74	0.0234
20	2.46	0.0331
30	3.33	0.0448

Auxiliary Information

Method/Apparatus/Procedure:

Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. R. Jones and C. B. Monk, J. Chem. Soc. 2633 (1963).

Variables:
Temperature: 25–35 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

Solubility of water in butylbenzene

t/°C	$10^4 \cdot$ mL (2)/mL (1)
25	3.5
30	4.1
35	4.9

Auxiliary Information

Method/Apparatus/Procedure:

In a thermostatted glass-stoppered flask 10–25 mL, (1) was shaken for at least 4 h with tritiated water (a few mL of HTO equivalent to ~2 mc/mL), decanted, a 5 mL aliquot reshaken for 4 h with 5 mL H_2O in a 10 mL flask, sampled and assayed with a Nuclear Enterprises type 8301 liquid scintillation counter. The two-stage process eliminates quenching effect (due to solvent) on the scintillator.

Source and Purity of Materials:

(1) Laboratory grade, dried over $CaCl_2$ and fractionally distilled.
(2) Not specified.

Estimated Error:
Solubility: ±5% to ±1% (average deviation).

References:

[1] *Vogel Practical Organic Chemistry* (Longmans, Green and Co., London, 1956).

Components:

(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of butylbenzene in water at 25 °C was reported to be 0.05 g (1)/L sln and 0.00037 mol (l)/L sln.

Assuming that 1.00 kg sln=1.00 L sln the mass percentage and mole fraction, x_1 , calculated by the compilers are 0.005 g (1)/100 g sln and $6.7 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:

(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. A. Massaldi and C. J. King, J. Chem. Eng. Data **18**, 393 (1973).

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

The solubility of butylbenzene in water at 25 °C was reported to be $1.32 \cdot 10^{-4}$ mol (l)/L sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00177 g (1)/100 g sln and $2.4 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

A technique based on head-space analysis by gas–liquid chromatography was developed to determine solubilities of sparing soluble organics. Saturated solutions need not be prepared in advance whereby phase separation problems are avoided, nor have liquid samples to be analyzed. This method is versatile enough to allow determination provided that the pure vapor pressure of the substances is known. The gas chromatograph was a Varian Aerograph Model 1740 with a flame ionization detector.

Source and Purity of Materials:

(1) Matheson Coleman and Bell Co., highest purity; used as received.
(2) Not specified.

Estimated Error:

Temperature: ±0.05 °C.

Components:

(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).

Variables:

Temperature: 7.0–45.0 °C

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of butylbenzene in water

$t/°C$	$10^4 \cdot$ mol (1)/L sln	$10^3 \cdot$ g (1)/100 g sln (compilers)	$10^6 \cdot x_1$ (compilers)
7.0	0.994±0.029	1.334	1.791
10.0	0.967±0.010	1.298	1.743
12.5	0.979±0.013	1.315	1.765
15.0	0.966±0.020	1.298	1.742
17.5	0.979±0.012	1.316	1.766
20.0	1.018±0.023	1.369	1.837
25.0	1.025±0.041	1.380	1.852
30.0	1.086±0.013	1.464	1.965
35.0	1.147±0.036	1.549	2.079
40.0	1.234±0.033	1.669	2.240
45.0	1.411±0.009	1.912	2.567

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were determined by the technique reported in May *et al.*[1] and DeVoe *et al.*[2] using an automated coupled-column liquid chromatographic apparatus, described in Owens *et al.*[3] A saturated solution was generated by pumping water through a column containing the solute coated on Chromosorb W. A known volume of the saturated solution was passed through a small extractor column filled with reverse phase packing where the solute was removed quantitatively. The extracted solute was then eluted with a water–methanol mixture, separated from impurities on an hplc analytical column, and analyzed by UV spectrophotometry at 254 nm. The standard deviation of the peak area for the known solution was <2.4%. 3–7 measurements at each temperature were made.

Source and Purity of Materials:

(1) Albany Internationals Chemicals Division; used as received; purity >99% by glc.
(2) hplc grade.

Estimated Error:

Temperature: ±0.05 °C.
Solubility: as above.

References:

[1] W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[2] H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[3] J. W. Owens, T. J. Buckley, and H. DeVoe, J. Res. Natl. Bur. Stand. (USA) **90**, 41 (1985).

Components:

(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

The solubility of butylbenzene in water at 25 °C was reported to be 11.8 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00118 g (1)/100 g sln and $1.58 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

The concentration of (1) in (2) was determined by gas chromatography.

Source and Purity of Materials:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 0.1 mg (1)/kg (2) (standard deviation of the mean for 6 replicates).

Components:	**Original Measurements:**
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of butylbenzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$1.03\cdot 10^{-4}$	$1.39\cdot 10^{-3}$	$1.86\cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with (1) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping (2) into the inlet of the coated column. The column effluent was then analyzed by hplc and glc. The column was thermostated by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:

(1) Source not specified; purity >99 mole % checked by high-temperature glc.
(2) Source not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:

[1] H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2] W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

2.4. *sec*-Butylbenzene+Water

Components:	**Evaluators:**
(1) *sec*-Butylbenzene; $C_{10}H_{14}$; [135-98-8] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of *sec*-Butylbenzene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Andrews and Keefer,[1] and Sutton and Calder[3] at 298 K.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1=\ln x_{1,\min}+D[(T_{\min}/T)\ln(T_{\min}/T)+1-(T_{\min}/T)], \tag{1}$$

where: $\ln x_{1,\min}=-12.79$; $D=51.15$; $T_{\min}=290$ K.

Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 8. The data of Sutton and Calder[3] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Andrews and Keefer[1] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in *sec*-Butylbenzene (1)

The experimental solubility data for (2) in (1) have been investigated by Englin *et al.*[2] at 283–303 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2=d_1+d_2(1/T_r-1)+d_3(1-T_r)^{1/3}+d_4(1-T_r), \tag{2}$$

where: $d_1=-0.268$; $d_2=-2.638$; $d_3=0.322$; $d_4=-7.077$; $T_r=T/582.7$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of *sec*-butylbenzene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 9. All the data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[4] are independent data. Therefore these data are Rejected.

References:

[1] L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[2] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[3] C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[4] T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

TABLE 8. Experimental values for solubility of *sec*-butylbenzene (1) in water (2)

T/K	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1\pm 30\%$
298.2	$4.15\cdot 10^{-6}$ (D; Ref. 1), $2.36\cdot 10^{-6}$ (T; Ref. 3)	$2.8\cdot 10^{-6}$

TABLE 9. Experimental values for solubility of water (2) in *sec*-butylbenzene (1)

T/K	Experimental values x_2 (D=doubtful)	Reference values $x_2 \pm 30\%$
283.2	$2.23 \cdot 10^{-3}$ (D; Ref. 2)	$1.6 \cdot 10^{-3}$
293.2	$3.13 \cdot 10^{-3}$ (D; Ref. 2)	$2.2 \cdot 10^{-3}$
303.2	$4.20 \cdot 10^{-3}$ (D; Ref. 2)	$2.9 \cdot 10^{-3}$

Components: (1) *sec*-Butylbenzene; $C_{10}H_{14}$; [135-98-8] (2) Water; H_2O; [7732-18-5]	**Original Measurements:** L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
Variables: One temperature: 25 °C	**Prepared By:** A. Maczynski and Z. Maczynska

Experimental Values

The solubility of *sec*-butylbenzene in water at 25 °C was reported to be 0.0309 g (1)/100 g sln.
The corresponding mole fraction, x_1 calculated by the compilers is $4.15 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was rotated for 24 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:

(1) Eastman Kodak Co. white label; fractionally distilled; boiling point range 175.0–175.8 °C.
(2) Not specified.

Estimated Error:

Not specified.

Components:
(1) *sec*-Butylbenzene; $C_{10}H_{14}$; [135-98-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 10–30 °C

Prepared By:
A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in *sec*-butylbenzene

t/°C	x_2 (compiler)	g (2)/100 g sln
10	0.00223	0.0226
20	0.00313	0.0317
30	0.00420	0.0426

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced to a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) *sec*-Butylbenzene; $C_{10}H_{14}$; [135-98-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of *sec*-butylbenzene in water at 25 °C was reported to be 17.6 mg (1)/kg (2).
The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00176 g (1)/100 g sln and $2.36 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:
The concentration of (1) in (2) was determined by gas chromatography.

Source and Purity of Materials:
(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 0.2 (standard deviation of the mean for 6 replicates).

2.5. tert-Butylbenzene+Water

Components:	**Evaluators:**
(1) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of *tert*-Butylbenzene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Andrews and Keefer,[1] and Sutton and Calder[3] at 298 K.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \qquad (1)$$

where $\ln x_{1,\min} = -13.05$; $D = 52.24$; $T_{\min} = 290$ K.

Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 10. All the data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in *tert*-Butylbenzene (1)

The experimental solubility data for (2) in (1) have been investigated by Englin *et al.*[2] at 283–303 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r) \qquad (2)$$

where $d_1 = -0.281$; $d_2 = -2.831$; $d_3 = 0.360$; $d_4 = -6.777$; $T_r = T/580.8$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of *tert*-butylbenzene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 11. The data of Englin[2] at 283 K are in good agreement (within 30% relative standarddeviation) with the reference data and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

References:

[1] L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[2] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[3] C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

TABLE 10. Experimental values for solubility of *tert*-butylbenzene (1) in water (2)

T/K	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
298.2	$4.60 \cdot 10^{-6}$ (D; Ref. 1), $3.95 \cdot 10^{-6}$ (D; Ref. 3)	$2.2 \cdot 10^{-6}$

TABLE 11. Experimental values for solubility of water (2) in *tert*-butylbenzene (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
283.2	$2.03 \cdot 10^{-3}$ (T; Ref. 2)	$1.6 \cdot 10^{-3}$
293.2	$2.88 \cdot 10^{-3}$ (D; Ref. 2)	$2.2 \cdot 10^{-3}$
303.2	$3.83 \cdot 10^{-3}$ (D; Ref. 2)	$2.9 \cdot 10^{-3}$

Components:	**Original Measurements:**
(1) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Values

The solubility of *tert*-butylbenzene in water at 25 °C was reported to be 0.0034 g (1)/100 g sln.

The corresponding mole fraction, x_1 calculated by the compilers is $4.6 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was rotated for 24 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:

(1) Eastman Kodak Co. white label; fractionally distilled; boiling point range 167.8–168.0 °C.
(2) Not specified.

Estimated Error:

Not specified.

Components:

(1) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:

Temperature: 10–30 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in tert-butylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	2.03	0.0205
20	2.88	0.0292
30	3.83	0.0389

Auxiliary Information

Method/Apparatus/Procedure:

Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:

(1) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

The solubility of *tert*-butylbenzene in water at 25 °C was reported to be 29.5 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00295 g (1)/100 g sln and $3.95 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

The concentration of (1) in (2) was determined by gas chromatography.

Source and Purity of Materials:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 0.3 (standard deviation of the mean for 6 replicates).

2.6. *p*-Cymene (1-methyl-4-(1-methylethyl)benzene)+Water

Components:	**Evaluators:**
(1) *p*-Cymene (1-methyl-4-(1-methylethyl)benzene); $C_{10}H_{14}$; [99-87-6] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of *p*-Cymene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Banerjee *et al.*,[1] Booth and Everson[2] at 298 K, and Miller and Hawthorne[4] at 298–473 K and 6000 kPa. Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \qquad (1)$$

where: $\ln x_{1,\min} = -13.13$; $D = 52.56$; $T_{\min} = 290$ K.

Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 12. The data of Miller and Hawthorne[4] at 423 and 473 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in *p*-Cymene (1)

The experimental solubility data for (2) in (1) have been investigated by Englin *et al.*[3] at 283–303 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r) \qquad (2)$$

where: $d_1 = -0.259$; $d_2 = -2.611$; $d_3 = 0.366$; $d_4 = -7.192$; $T_r = T/584.0$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of *p*-cymene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed.

The experimental and reference solubility data for (2) in (1) are listed in Table 13 and shown in Fig. 5. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:

[1] S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
[2] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
[3] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[4] D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).

TABLE 12. Experimental values for solubility of *p*-cymene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
298.0	6000 (Ref. 4)	$3.00 \cdot 10^{-6}$ (D; Ref. 4)	$2.0 \cdot 10^{-6}$
298.2		$3.13 \cdot 10^{-6}$ (D; Ref. 1), $5.00 \cdot 10^{-5}$ (D; Ref. 2)	$2.0 \cdot 10^{-6}$
323.0	6000 (Ref. 4)	$4.00 \cdot 10^{-6}$ (D; Ref. 4)	$2.7 \cdot 10^{-6}$
373.0	6000 (Ref. 4)	$1.10 \cdot 10^{-5}$ (D; Ref. 4)	$8.2 \cdot 10^{-6}$
423.0	6000 (Ref. 4)	$4.30 \cdot 10^{-5}$ (T; Ref. 4)	$3.7 \cdot 10^{-5}$
473.0	6000 (Ref. 4)	$2.00 \cdot 10^{-4}$ (T; Ref. 4)	$1.9 \cdot 10^{-4}$

TABLE 13. Experimental values for solubility of water (2) in *p*-cymene (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
283.2	$1.66 \cdot 10^{-3}$ (T; Ref. 3)	$1.6 \cdot 10^{-3}$
293.2	$2.27 \cdot 10^{-3}$ (T; Ref. 3)	$2.2 \cdot 10^{-3}$
303.2	$3.08 \cdot 10^{-3}$ (T; Ref. 3)	$2.9 \cdot 10^{-3}$

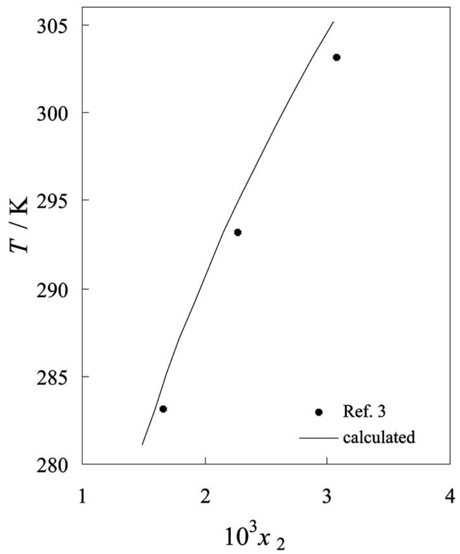

FIG. 5. All the solubility data for water (2) in *p*-cymene (1).

Components:
(1) *p*-Cymene; $C_{10}H_{14}$; [99-87-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

Variables:
One temperature: 25 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of *p*-cymene in water was reported to be $1.74\cdot 10^{-4}$ mol/L sln.

Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction, x_1 , solubilities, calculated by the compiler, are $2.34\cdot 10^{-3}$ g (1)/100 g sln and $3.13\cdot 10^{-6}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of *p*-cymene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25±0.2 °C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10 000 rpm for 60 min. in a head pre-equilibrated to 25±0.3 °C, following which aliquots of the solution were removed for analysis by GC after exhaustive extraction with hexane. A HP 5370A (FID) instrument and a 3% OV-1 on Chromosorb W column was used. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

Source and Purity of Materials:
(1) Aldrich; purity not specified.
(2) Distilled.

Estimated Error:
Temperature: ±0.2 °C.
Solubility: ±3.1% rel. (representing 1 standard deviation)

Components:
(1) *p*-Cymene; $C_{10}H_{14}$; [99-87-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of *p*-cymene in water at 25 °C was reported to be 0.04 g (1)/100 mL (2).

Assuming a solution density of 1.00, the mass percentage and mole fraction, x_1 , calculated by the compilers are 0.04 g (1)/100 g sln and $5\cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

Stoppered Babcock tubes with necks graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in a constant-temperature water bath and weighed quantities of (1) were added to this solution. The mixture was then shaken for 5 min, returned to the bath for a minimum of 10 min, and then centrifuged for 5 min. After this treatment, this volume of residue was determined directly.

Source and Purity of Materials:
(1) Source not specified; CP or highest commercial grade; used as received.
(2) Distilled.

Estimated Error:
Solubility: ±0.1 mL (1)/100 mL (2).

Components:

(1) *p*-Cymene; $C_{10}H_{14}$; [99-87-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:

Temperature: 10–30 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in *p*-cymene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	1.66	0.0223
20	2.27	0.0305
30	3.08	0.0415

Auxiliary Information

Method/Apparatus/Procedure:

Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:

(1) *p*-Cymene; $C_{10}H_{14}$; [99-87-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).

Variables:

Temperature: 298.0–473.0 K
Pressure: 60 bar

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of *p*-cymene in water

T/K	P/bar	g (1)/100 g sln (compilers)	$10^4 \cdot x_1$
298.0	60	$2.23 \cdot 10^{-5}$	0.030 ± 0.002
323.0	60	$2.98 \cdot 10^{-5}$	0.040 ± 0.004
373.0	60	$8.19 \cdot 10^{-5}$	0.11 ± 0.01
423.0	60	$3.20 \cdot 10^{-4}$	0.43 ± 0.02
473.0	60	$1.49 \cdot 10^{-3}$	2.0 ± 0.2

Auxiliary Information

Method/Apparatus/Procedure:

The dynamic method described in Miller and Hawthorne[1] was used. A high-pressure saturation cell was filled with component (1) and placed in the oven of gas chromatograph to provide precise temperature control. Next water was pumped into the saturation cell. After a 60 min equilibration 10 fractions were collected for 3 min each. The details of filling procedure, equilibration, and sampling were described in the paper. The analyses were performed using an HP model 5890 gas chromatograph with flame ionization detection.

Source and Purity of Materials:

(1) Sigma-Aldrich, Milwaukee, WI; purity >99%; used as received.
(2) Not stated.

Estimated Error:

Temperature: ±0.1 K.
Solubility: as above.

References:

[1] D. J. Miller and S. B. Hawthorne, Anal. Chem. **70**, 1618 (1998).

2.7. Diethylbenzene+Water

Components:

(1) Diethylbenzene; $C_{10}H_{14}$; [25340-17-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:

Temperature: 0–50 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in diethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
0	1.57	0.0159
10	2.23	0.0226
20	3.15	0.0319
30	4.25	0.0431
40	5.65	0.0574
50	7.43	0.0756

Auxiliary Information

Method/Apparatus/Procedure:

Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

2.8. 1,2-Diethylbenzene+Water

Components:

(1) 1,2-Diethylbenzene; $C_{10}H_{14}$; [135-01-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Ben-Naim and J. Wilf, J. Phys. Chem. **70**, 771 (1979).

Variables:

Temperature: 10.0 and 20.0 °C

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1,2-diethylbenzene in water

t/°C	$10^4 \cdot$ mol (1)/L sln	$10^3 \cdot$ g (1)/100 g sln (compilers)	$10^6 \cdot x_1$ (compilers)
10.0	5.3	7.2	9.6
20.0	5.3	7.2	9.6

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A saturated solution was diluted several times and the optical density was measured by a Perkin-Elmer Model 450 spectrophotometer in the UV region of 200–400 m.

Source and Purity of Materials:

(1) Fluka, purum grade, purity ⩾95%; used as received.
(2) Triply distilled.

Estimated Error:

Temperature: ±0.2 °C
Solubility: 1% (reproducibility of measurements).

2.9. 1,3-Diethylbenzene+Water

Components:
(1) 1,3-Diethylbenzene; $C_{10}H_{14}$; [141-93-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Variables:
Temperature: 310.93–582.54 K
Pressure: 0.5081–11.714 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1,3-diethylbenzene in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^3 \cdot x_1$
310.93	—	0.003203	0.00430
366.48	—	0.00745	0.0100
422.04	0.5081	0.03203	0.0430
477.59	1.8912	0.2008	0.270
533.15	5.405	1.158	1.57
549.82	7.074	2.243	3.07

Solubility of water in 1,3-diethylbenzene

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
310.93	—	0.0460	0.00342
366.48	—	0.221	0.0162
422.04	0.5081	0.839	0.0593
477.59	1.8912	2.44	0.157
533.15	5.405	7.22	0.367
549.82	7.074	10.15	0.457
582.54[a]	11.714	31.74	0.776

[a] Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of (1) in (2) was measured by glc, while that of (2) in (1) by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus. Data other than three-phase critical end point were previously reported in Brady *et al.*[3]

Source and Purity of Materials:
(1) Aldrich; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:
Temperature: ±0.6 K at critical end point.[a]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[a]
Pressure: 1% and ±0.04 MPa at critical end point.[a]

References:
[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).
[3] C. J. Brady, J. R. Cunningham, and G. M. Wilson, GPA/API Res. Proj. RR-62, Gas Processors Assoc., Tulsa, OK (1982).

2.10. 1,4-Diethylbenzene+Water

Components:
(1) 1,4-Diethylbenzene; $C_{10}H_{14}$; [105-05-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Ben-Naim and J. Wilf, J. Phys. Chem. **70**, 771 (1979).

Variables:
Temperature: 10.0 and 20.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1,4-diethylbenzene in water

t/°C	$10^4 \cdot$ mol (1)/L sln	$10^3 \cdot$ g (1)/100 g sln (compilers)	$10^6 \cdot x_1$ (compilers)
10.0	1.85	2.48	3.33
20.0	1.85	2.48	3.33

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A saturated solution was diluted several times and the absorbance was measured by a Perkin-Elmer Model 450 spectrophotometer in the UV region of 200–400 m.

Source and Purity of Materials:
(1) Fluka, purum grade, purity ⩾95%; used as received.
(2) Triply distilled.

Estimated Error:
Temperature: ±0.2 °C
Solubility: 1% (reproducibility of measurements).

2.11. Isobutylbenzene+Water

Components:	**Original Measurements:**
(1) Isobutylbenzene; $C_{10}H_{14}$; [538-93-2] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of isobutylbenzene in water at 25 °C and at system pressure was reported to be 10.1 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0101 g (1)/100 g sln and $1.35 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±1 °C.
Solubility: ±0.4 mg (1)/kg (2).

2.12. 1,2,4,5-Tetramethylbenzene+Water

Components:	**Original Measurements:**
(1) 1,2,4,5-Tetramethylbenzene; $C_{10}H_{14}$; [95-93-2] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 1,2,4,5-tetramethylbenzene in water at 25 °C and at system pressure was reported to be 3.48 mg (1)/kg (2).

The corresponding mass per cent and mole fraction, x_1, calculated by the compiler are $3.48 \cdot 10^{-4}$ g (1)/100 g sln and $4.67 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2–4 days. Analyses were carried out using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±1 °C.
Solubility: ±0.28 mg (1)/kg (2).

2.13. *d*-Limonene+Water

Components:	**Evaluators:**
(1) *d*-Limonene (4-isopropenyl-1-methylcyclohexane); $C_{10}H_{16}$; [5989-27-5] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of *d*-Limonene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Massaldi and King[1] at 273–298 K and Miller and Hawthorne[2] at 298–473 K.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{s\ \ln} C_p / \mathrm{R})[\mathrm{T}_{\min}/T - \ln(T_{\min}/T) - 1], \quad (1)$$

where: $\ln x_{1,\min} = -14.11$; $\Delta_{\sin} C_p / R = 63.0$; $T_{\min} = 298$ K.

Equation (1) is based on all available solubility data of unsaturated hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference data of Massaldi and King[1] and Miller and Hawthorne[2] are listed in Table 14. The data of Miller and Hawthorne[2] at 423 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

References:

[1] H. A. Massaldi and C. J. King, J. Chem. Eng. Data **18**, 393 (1973).

[2] D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 315 (2000).

TABLE 14. Experimental values for solubility of *d*-limonene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2		$1.3 \cdot 10^{-6}$ (D; Ref. 1)	$9.6 \cdot 10^{-7}$
278.2		$1.4 \cdot 10^{-6}$ (D; Ref. 1)	$8.7 \cdot 10^{-7}$
298.0	7000 (Ref. 2)	$1.0 \cdot 10^{-6}$ (D; Ref. 2)	$7.5 \cdot 10^{-7}$
298.2		$1.8 \cdot 10^{-6}$ (D; Ref. 1)	$7.5 \cdot 10^{-7}$
323.0	7100 (Ref. 2)	$1.3 \cdot 10^{-6}$ (D; Ref. 2)	$9.1 \cdot 10^{-7}$
373.0	7200 (Ref. 2)	$4.3 \cdot 10^{-6}$ (D; Ref. 2)	$3.3 \cdot 10^{-6}$
423.0	7000 (Ref. 2)	$2.1 \cdot 10^{-5}$ (T; Ref. 2)	$2.4 \cdot 10^{-5}$
473.0	6900 (Ref. 2)	$5.7 \cdot 10^{-5}$ (D; Ref. 2)	$2.5 \cdot 10^{-4}$

Components:	**Original Measurements:**
(1) *d*-Limonene; $C_{10}H_{16}$; [5989-27-5] (2) Water; H_2O; [7732-18-5]	H. A. Massaldi and C. J. King, J. Chem. Eng. Data **18**, 393 (1973).
Variables:	**Prepared By:**
Temperature: 0–25 °C	A. Maczynski and Z. Maczynska

Experimental Values

Solubility of *d*-limonene in water

T/°C	$10^6 \cdot x_1$	$10^3 \cdot$ g (1)/100 g sln (compiler)	mg (1)/L sln	$10^4 \cdot$ mol (1)/L sln
0	1.3	0.97	9.7	0.708
5	1.4	1.04	10.4	0.767
25	1.8	1.38	13.8	1.013

Auxiliary Information

Method/Apparatus/Procedure:

A technique based on head-space analysis by glc was developed to determine solubilities of sparingly soluble organics. Saturated solutions need not be prepared in advance whereby phase separation problems are avoided, nor have liquid samples to be analyzed. This method is versatile enough to allow determinations provided that the pure vapor pressure of the substances is known. The gas chromatograph was a Varian Aerograph Model 1740 with a flame ionization detector.

Source and Purity of Materials:

(1) Matheson Coleman and Bell Co., highest purity; kept under N_2 atmosphere at −2 °C in a dark container; used as received.

(2) Not specified.

Estimated Error:

Temperature: ±0.05 °C.

Components:	**Original Measurements:**
(1) *d*-Limonene; $C_{10}H_{16}$; [5989-27-5] (2) Water; H_2O; [7732-18-5]	D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 315 (2000).
Variables:	**Prepared By:**
Temperature: 298.0–473.0 K Pressure: 69–72 bar	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of *d*-limonene in water

T/K	P/bar	g (1)/100 g sln (compilers)	$10^5 \cdot x_1$
298.0	70	0.00076	0.10±0.01
323.0	71	0.00098	0.13±0.01
373.0	72	0.00325	0.43±0.01
423.0	70	0.0159	2.1±0.1
473.0	69	0.0431	5.7±0.2

Auxiliary Information

Method/Apparatus/Procedure:

The dynamic method described in Miller and Hawthorne[1] was used. A high-pressure saturation cell was filled with component (1) and place in the oven of a gas chromatograph to provide precise temperature control. Next water was pumped into the saturation cell. After a 60 min equilibration 10 fractions were collected for 3 min each. The details of filling procedure, equilibration, and sampling were described in the paper. The analyses were performed using an HP model 5890 gas chromatograph with flame ionization detection.

Source and Purity of Materials:

(1) Sigma-Aldrich, Milwaukee, WI; purity >97%; used as recieved.
(2) Not stated.

Estimated Error:

Temperature: ±0.1 K.
Solubility as above.

Reference:

[1] D. J. Miller and S. B. Hawthorne, Anal. Chem. **70**, 1618 (1998).

2.14. *cis*- and *cis*+*trans* Bicyclo[4.4.0]decane+Water

Components:	**Evaluators:**
(1) *cis*-Bicyclo[4.4.0]decane (*cis*-decalin, *cis*-decahydronaphthalene); $C_{10}H_{18}$; [493-01-06] or *cis* +*trans* Bicyclo[4.4.0]decane (*cis*+*trans* decalin, *cis* +*trans* decahydronaphthalene); $C_{10}H_{18}$; [91-17-8] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of *cis* and *cis*+*trans* Bicycle[4.4.0]decane (1) in Water (2)

Cis and *cis*+*trans* bicycle[4.4.0]decane have been evaluated together. Our experience is that generally isomers do not differ in respect to the solubility.

The experimental solubility data for (1) in (2) have been investigated by Booth and Everson[1] and Price[5] at 298 K and Economou *et al.*[2] at 374–576 K and 110–10 273 kPa.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\mathrm{min}} + (\Delta_{s\,\ln} C_p / R)[T_{\mathrm{min}}/T - \ln(T_{\mathrm{min}}/T) - 1], \qquad (1)$$

where: $\ln x_{1,\mathrm{min}} = -15.96$; $\Delta_{\mathrm{sln}} C_p/R = 60.5$; $T_{\mathrm{min}} = 298$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories

All the experimental and reference data are listed in Table 15 and shown in Fig. 6. The data of Economou *et al.*[2] at 374 K and Price[5] at 298 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in *cis* and *cis*+*trans* Bicycle[4.4.0]decane (1)

The experimental solubility data for (2) in (1) have been investigated by Economou *et al.*[2] at 374–576 K and 110–10 273 kPa and Englin *et al.*[3] at 293–313 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \qquad (2)$$

where: $d_1 = -0.120$; $d_2 = -6.030$; $d_3 = -1.919$; $d_4 = 0.221$; $T_r = T/605.9$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of *cis* and *cis*+*trans* bicyclo[4.4.0]decane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 16 and shown in Fig. 7. The data of Economou *et al.*[2] at 424–576 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Rejected and Inaccessible Data

The data reported by Jockers *et al.*[4] at 613–673 K and 18 000–71 000 kPa lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
[2] I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
[3] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[4] R. Jockers, R. Paas, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **81**, 1093 (1977).
[5] L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

TABLE 15. Experimental values for solubility of *cis* and *cis*+*trans* bicyclo[4.4.0]decane (1) in water (2)

T/K	P/kPa	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
298.2		$2.30 \cdot 10^{-5}$ (D; Ref. 1), $1.16 \cdot 10^{-7}$ (T; Ref. 5)	$1.3 \cdot 10^{-7}$
374.2	110 (Ref. 2)	$4.10 \cdot 10^{-7}$ (T; Ref. 2)	$5.7 \cdot 10^{-7}$
424.7	547 (Ref. 2)	$2.00 \cdot 10^{-6}$ (D; Ref. 2)	$3.9 \cdot 10^{-6}$
475.2	1689 (Ref. 2)	$7.70 \cdot 10^{-6}$ (D; Ref. 2)	$3.8 \cdot 10^{-5}$
576.2	10 273 (Ref. 2)	$8.80 \cdot 10^{-5}$ (D; Ref. 2)	$5.7 \cdot 10^{-3}$

TABLE 16. Experimental values for solubility of water (2) in *cis* and *cis*+*trans* bicyclo[4.4.0]decane (1)

T/K	P/kPa	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
293.2		$4.84 \cdot 10^{-4}$ (D; Ref. 3)	$3.4 \cdot 10^{-4}$
303.2		$8.06 \cdot 10^{-4}$ (D; Ref. 3)	$5.2 \cdot 10^{-4}$
313.2		$1.258 \cdot 10^{-3}$ (D; Ref. 3)	$7.8 \cdot 10^{-4}$
374.2	110 (Ref. 2)	$9.70 \cdot 10^{-3}$ (D; Ref. 2)	$5.7 \cdot 10^{-3}$
424.7	547 (Ref. 2)	$2.53 \cdot 10^{-2}$ (T; Ref. 2)	$2.0 \cdot 10^{-2}$
451.2		$4.05 \cdot 10^{-2}$ (T; Ref. 2)	$3.5 \cdot 10^{-2}$
475.2	1689 (Ref. 2)	$5.40 \cdot 10^{-2}$ (T; Ref. 2)	$5.6 \cdot 10^{-2}$
576.2	10 273 (Ref. 2)	$3.09 \cdot 10^{-1}$ (T; Ref. 2)	$3.3 \cdot 10^{-1}$

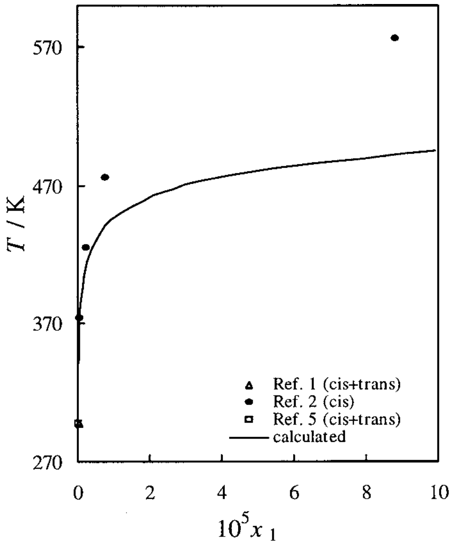

FIG. 6. All the solubility data for *cis* and *cis*+*trans* bicyclo[4.4.0]decane (1) in water (2).

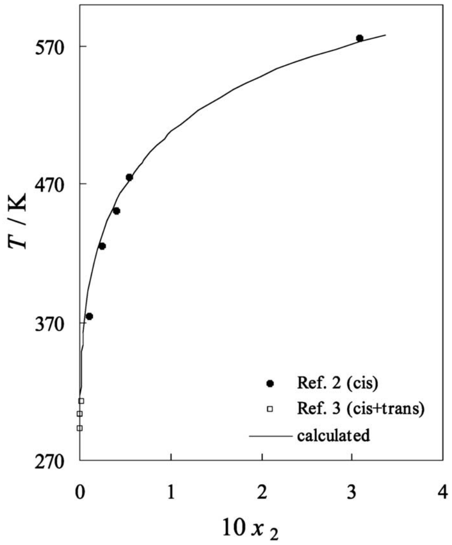

FIG. 7. All the solubility data for water (2) in *cis* and *cis*+*trans* bicyclo[4.4.0]decane (1).

Components:

(1) *cis+trans* Bicyclo[4.4.0]decane (*cis+trans* decalin, *cis* *+trans* decahydronaphthalene); $C_{10}H_{18}$; [91-17-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. S. Booth and H. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

Variables:

One temperature: 25 °C

Prepared By:

G. T. Hefter

Experimental Values

The solubility of *cis+trans* bicyclo[4.4.0]decane in water at 25 °C was reported to be <0.02 mL (1)/100 mL (2).

A similar result was reported for (1) in 40.0% (w/w?) aqueous sodium xylene sulfonate.

Auxiliary Information

Method/Apparatus/Procedure:

A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.03 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath and then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute, measured directly in the tube, from the total added.

Source and Purity of Materials:

(1) Highest grade commercial sample available; no other details given.
(2) Distilled.

Estimated Error:

Not specified.

Components:

(1) *cis+trans* Bicyclo[4.4.0]decane (*cis+trans* decalin, *cis* *+trans* decahydronaphthalene); $C_{10}H_{18}$; [91-17-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:

Temperature: 20–40 °C

Prepared By:

A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in *cis+trans* bicyclo[4.4.0]decane

$t/°C$	$10^4 \cdot x_2$ (compiler)	g (2)/100 g sln
20	4.84	0.0063
30	8.06	0.0105
40	12.58	0.0164

Auxiliary Information

Method/Apparatus/Procedure:

Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) *cis+trans* Bicyclo[4.4.0]decane (*cis+trans* decalin, *cis +trans* decahydronaphthalene); $C_{10}H_{18}$; [91-17-8] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of *cis+trans* bicycle[4,4,0]decane in water at 25 °C and at system pressure was reported to be 0.889 mg (1)/kg (2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $8.89 \cdot 10^{-5}$ g (1)/100 g sln and $1.16 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±1 °C.
Solubility: ±0.031 mg (1)/kg (2).

2.15. *cis*-Bicyclo[4.4.0]decane+Water

Components:	**Original Measurements:**
(1) *cis*-Bicyclo[4.4.0]decane (*cis*-decalin, *cis*-decahydronaphthalene); $C_{10}H_{18}$; [493-01-6] (2) Water; H_2O; [7732-18-5]	I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
Variables:	**Prepared By:**
Temperature: 374.15–599.09 K Pressure: 0.110–14.438 MPa	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of *cis*-bicyclo[4.4.0]decane in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^5 \cdot x_1$
374.15	0.110	0.000315	0.041
424.65	0.5468	0.00153	0.20
475.15	1.689	0.00591	0.77
576.15	10.273	0.0675	8.8

Solubility of water in *cis*-bicyclo[4.4.0]decane

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
374.15	0.110	0.1275	0.00970
424.65	0.5468	0.337	0.0253
451.15	—	0.547	0.0405
475.15	1689	0.738	0.0540
576.15	10273	5.51	0.309
599.09[a]	14438	33.03	0.791

[a] Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of hydrocarbon in water was measured by glc, while that of water in hydrocarbon by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus.

Source and Purity of Materials:

(1) Aldrich; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:

Temperature: ±0.6 K at critical end point.[a]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[a]
Pressure: 1% and ±0.04 MPa at critical end point.[a]

References:

[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

Components:

(1) *cis*-Bicyclo[4.4.0]decane (*cis*-decalin, *cis*-decahydronaphthalene); $C_{10}H_{18}$; [493-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. Jockers, R. Paas, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **81**, 1093 (1977).

Variables:

Temperature: 324.0–400.0 °C
Pressure: 180–710 bar

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Critical data of *cis*-bicyclo[4.4.0]decane and water

t/°C	P/bar
340.0[a]	180
350.0	230
360.0	302
370.0	388
380.0	478
390.0	590
400.0	710

[a] Critical end point of three-phase (liquid-liquid-gas) line.

Auxiliary Information

Method/Apparatus/Procedure:

The measurements on *cis*-bicyclo[4.4.0]decane–water mixtures were made in an optical high temperature high pressure autoclave with magnetic stirring described in Alwani and Schneider.[1] No more details were reported in the paper.

Source and Purity of Materials:

(1) Not stated
(2) Not stated.

Estimated Error:

Not stated.

References:

[1] Z. Alwani and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **73**, 294 (1969).

2.16. 1-Butylcyclohexane+Water

Components:

(1) Butylcyclohexane; $C_{10}H_{20}$; [1678-93-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Variables:

Temperature: 310.93–584.32 K
Pressure: 0.5068–11.845 MPa

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of butylcyclohexane in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^4 \cdot x_1$
366.48	—	0.000148	0.0019
422.04	0.5068	0.00156	0.020
477.59	1.9023	0.00125	0.16
533.15	5.4220	0.1524	1.96
549.82	7.1078	0.3284	4.23

Solubility of water in butylcyclohexane

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
310.93	—	0.00950	0.000739
366.48	—	0.0792	0.00613
422.04	0.5068	0.378	0.0287
477.59	1.9023	1.42	0.101
533.15	5.4220	4.45	0.266
549.82	7.1078	6.39	0.347
584.32[a]	11.845	27.81	0.750

[a] Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of (1) in (2) was measured by glc, while that of (2) in (1) by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus. Data other than three-phase critical end point were previously reported in Brady *et al.*[3]

Source and Purity of Materials:

(1) Pfaltz and Bauer; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:

Temperature: ±0.6 K at critical end point.[a]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[a]
Pressure: 1% and ±0.04 MPa at critical end point.[a]

References:

[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).
[3] C. J. Brady, J. R. Cunningham, and G. M. Wilson, GPA/API Res. Proj. RR-62, Gas Processors Assoc., Tulsa, OK (1982).

2.17. 1-Decene+Water

Components:	**Evaluators:**
(1) 1-Decene; $C_{10}H_{20}$; [872-05-9] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of 1-Decene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Economou *et al.*[1] at 374–576 K and 121–11 360 kPa, and Natarajan and Venkatachalam[2] at 288–298 K.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\mathrm{min}} + (\Delta_{\mathrm{sln}} C_p / R)[T_{\mathrm{min}}/T - \ln(T_{\mathrm{min}}/T) - 1] \qquad (1)$$

where: $\ln x_{1,\mathrm{min}} = -18.21$; $\Delta_{\mathrm{sln}} C_p / R = 78.4$; $T_{\mathrm{min}} = 306$ K.

Equation (1) is based on all available solubility data of unsaturated hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference data of Economou *et al.*[1] and Natarajan and Venkatachalam[2] are listed in Table 17. All the data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in 1-Decene (1)

The experimental solubility data for (2) in (1) have been investigated by Economou *et al.*[1] at 374–576 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r) \qquad (2)$$

where: $d_1 = 0.160$; $d_2 = -3.339$; $d_3 = -0.639$; $d_4 = -6.273$; $T_r = T/577.2$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1-decene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 18 and shown in Fig. 8. The data of Economou *et al.*[1] at 374–475 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Economou *et al.*[1] at 576 K are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

References:

[1] I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

[2] G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).

TABLE 17. Experimental values for solubility of 1-decene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
288.2		$1.5 \cdot 10^{-6}$ (D; Ref. 2)	$1.4 \cdot 10^{-8}$
293.2		$1.1 \cdot 10^{-6}$ (D; Ref. 2)	$1.3 \cdot 10^{-8}$
298.2		$7.3 \cdot 10^{-7}$ (D; Ref. 2)	$1.3 \cdot 10^{-8}$
374.2	121 (Ref. 1)	$5.1 \cdot 10^{-7}$ (D; Ref. 1)	$5.5 \cdot 10^{-8}$
424.7	552 (Ref. 1)	$1.4 \cdot 10^{-6}$ (D; Ref. 1)	$5.5 \cdot 10^{-7}$
475.2	1840 (Ref. 1)	$4.3 \cdot 10^{-6}$ (D; Ref. 1)	$9.0 \cdot 10^{-6}$
576.2	11 360 (Ref. 1)	$5.5 \cdot 10^{-5}$ (D; Ref. 1)	$4.7 \cdot 10^{-3}$

TABLE 18. Experimental values for solubility of water (2) in 1-decene (1)

T/K	P/kPa	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
374.2	121 (Ref. 1)	$1.33 \cdot 10^{-2}$ (T; Ref. 1)	$1.3 \cdot 10^{-2}$
424.2	552 (Ref. 1)	$4.22 \cdot 10^{-2}$ (T; Ref. 1)	$4.5 \cdot 10^{-2}$
475.2	1840 (Ref. 1)	$1.28 \cdot 10^{-1}$ (T; Ref. 1)	$1.3 \cdot 10^{-1}$
576.2	11 360 (Ref. 1)	$5.93 \cdot 10^{-1}$ (D; Ref. 1)	1.1

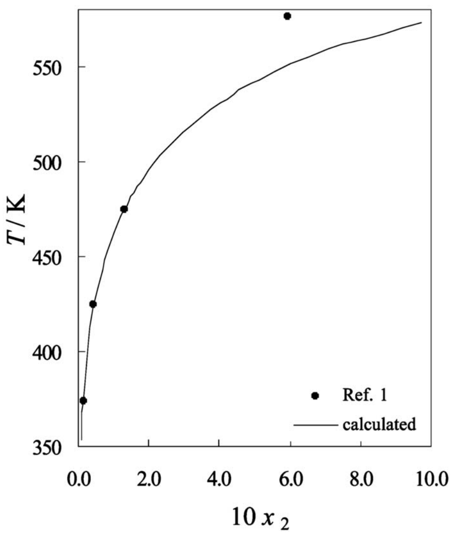

FIG. 8. All the solubility data for water (2) in 1-decene (1).

Components:	**Original Measurements:**
(1) 1-Decene; $C_{10}H_{20}$; [872-05-9] (2) Water; H_2O; [7732-18-5]	I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
Variables:	**Prepared By:**
Temperature: 374.15–576.15 K Pressure: 0.121–11.36 MPa	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1-decene in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^5 \cdot x_1$
374.15	0.121	0.000397	0.051
424.65	0.552	0.00109	0.14
475.15	1.84	0.00335	0.43
576.15[a]	11.36	0.0428	5.5

Solubility of water in 1-decene

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
374.15	0.121	0.173	0.0133
424.65	0.552	0.563	0.0422
475.15	1.84	1.85	0.128
576.15[a]	11.36	15.76	0.593
568.98[b]	9.942	23.06	0.700

[a] Above three-phase critical end point.

[b] Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of (1) in (2) was measured by glc, while that of (2) in (1) by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus.

Source and Purity of Materials:

(1) Aldrich; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:

Temperature: ±0.6 K at critical end point.[b]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[b]
Pressure: 1% and ±0.04 MPa at critical end point.[b]

References:

[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

Components:	**Original Measurements:**
(1) 1-Decene; $C_{10}H_{20}$; [872-05-9] (2) Water; H_2O; [7732-18-5]	G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).
Variables:	**Prepared By:**
Temperature: 15–25 °C	M. C. Haulait-Pirson and G. T. Hefter

Experimental Values

Solubility of 1-decene in 0.001 mol/L HNO_3 sln.

t/°C	$10^6 \cdot x_1$ (compiler)	$10^3 \cdot$ g (1)/100 g sln[b] (compiler)	10^5 mol (1)/L sln[a]
15	1.5	1.1	8.2
20	1.1	0.85	6.1
25	0.73	0.57	4.1

[a] Uncertainties stated to be ‘‘standard deviations from mean.’’

[b] Assuming a solution density of 1.00 g/mL at all temperatures.

Compiler’s note:

Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause the solubility of (1) to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol/L HCl.

Auxiliary Information

Method/Apparatus/Procedure:

15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the (1) content determined by titration with bromine using standard procedures.

Source and Purity of Materials:

(1) BDH: 99%.
(2) Not specified.

Estimated Error:

Temperature: ±0.05 °C.
Solubility: see table above.

2.18. Pentylcyclopentane+Water

Components:

(1) Pentylcyclopentane; $C_{10}H_{20}$; [3741-00-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of pentylcyclopentane in water at 25 °C and at system pressure was reported to be 0.115 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler was $1.15\cdot 10^{-5}$ g (1)/100 g sln and $1.5\cdot 10^{-8}$.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±1 °C.
Solubility: ±0.011 mg (1)/kg (2).

2.19. Decane+Water

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Evaluators:

A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of Decane (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Baker[1]	298	Hellinger and Sandler[6]	298
Baker[2]	298	Krasnoshchekova and Gubergrits[7]	298
Becke and Quitzsch[3]	293	Mackay *et al.*[8]	298
Economou *et al.*[4]	374–576 (124–11 238 kPa)	McAuliffe[9]	298
Franks[5]	298		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1=\ln x_{1,\min}+(\Delta_{s\ \ln}C_p/R)[T_{\min}/T-\ln(T_{\min}/T)-1], \tag{1}$$

where: $\ln x_{1,\min}=-19.72$; $\Delta_{\mathrm{sln}}C_p/R=79.7$; $T_{\min}=306$ K.

Equation (1) is based on all available solubility data of saturated hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 19. The data of Becke and Quitzsch[3] at 293 K, and Franks[5] at 298 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in Decane (1)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Becke and Quitzsch[3]	293	Namiot *et al.*[10]	423–563 (520–9360 kPa)
Economou *et al.*[4]	374–576 (124–11 238 kPa)	Schatzberg[11]	298 and 313
Hellinger and Sandler[6]	298		

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2=d_1+d_2(1/T_r-1)+d_3(1-T_r)^{1/3}+d_4(1-T_r), \tag{2}$$

where: $d_1=-0.087$; $d_2=-5.338$; $d_3=-0.910$; $d_4=-3.269$; $T_r=T/577.2$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of decane in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 20 and shown in Fig. 9. The data of Economou *et al.*,[4] Hellinger and Sandler,[6] Namiot *et al.*,[10] and Skripka[11] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Becke and Quitzsch[3] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

High Pressure Solubility of Decane (1) in Water (2)

The experimental high pressure solubility of (1) in (2) investigated by Skripka[12] at 498–563 K and 2900–78 500 kPa, and Wang and Chao[13] at 573–613 K and 9200–23 100 kPa have not been critically evaluated.

Rejected and Inaccessible Data

The data reported Roof[14] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1] E. G. Baker, Amer. Chem. Soc., Div. Petrol. Chem., Prepr. 3, No. 4, C-61 (1958).
[2] E. G. Baker, Science **129**, 871 (1959).
[3] A. Becke and G. Quitzsch, Chem. Tech. (Leipzig) **29**, 49 (1977).
[4] I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
[5] F. Franks, Nature (London) **210**, 87 (1966).
[6] S. Hellinger and S. I. Sandler, J. Chem. Eng. Data **40**, 321 (1995).
[7] P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).
[8] D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. **573**, 251 (1975).
[9] C. McAuliffe, Science **163**, 478 (1969).
[10] A. Yu. Namiot, V. G. Skripka, and Yu. G. Lotter, Zh. Fiz. Khim. **50**, 2718 (1976).
[11] P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).
[12] V. G. Skripka, Tr., Vses. Neftegazov. Nauch.-Issled. Inst. **61**, 139 (1976).
[13] Q. Wang and K.-C. Chao, Fluid Phase Equilib. **59**, 207 (1990).
[14] J. G. Roof, J. Chem. Eng. Data **15**, 301 (1970).

TABLE 19. Experimental values for solubility of decane (1) in water (2)

T/K	P/kPa	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
293.2		$2.50 \cdot 10^{-9}$ (T; Ref. 3)	$3.5 \cdot 10^{-9}$
298.2		$2.00 \cdot 10^{-9}$ (D; Ref. 1), $2.00 \cdot 10^{-9}$ (D; Ref. 2), $2.50 \cdot 10^{-9}$ (T; Ref. 5), $6.27 \cdot 10^{-9}$ (D; Ref. 6), $6.13 \cdot 10^{-9}$ (D; Ref. 6), $1.10 \cdot 10^{-9}$ (D; Ref. 7), $1.60 \cdot 10^{-7}$ (D; Ref. 8), $6.58 \cdot 10^{-9}$ (D; Ref. 9)	$3.3 \cdot 10^{-9}$
374.2	124 (Ref. 4)	$1.20 \cdot 10^{-7}$ (D; Ref. 4)	$1.5 \cdot 10^{-8}$
424.7	531 (Ref. 4)	$3.30 \cdot 10^{-7}$ (D; Ref. 4)	$1.5 \cdot 10^{-7}$
475.2	1779 (Ref. 4)	$1.40 \cdot 10^{-6}$ (D; Ref. 4)	$2.6 \cdot 10^{-6}$
576.2	11 238 (Ref. 4)	$4.90 \cdot 10^{-5}$ (D; Ref. 4)	$1.5 \cdot 10^{-3}$

TABLE 20. Experimental values for solubility of water (2) in decane (1)

T/K	P/kPa	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
293.2		$2.30 \cdot 10^{-3}$ (D; Ref. 3)	$5.1 \cdot 10^{-4}$
298.2		$5.20 \cdot 10^{-4}$ (T; Ref. 6), $5.40 \cdot 10^{-4}$ (T; Ref. 6), $5.70 \cdot 10^{-4}$ (T; Ref. 11)	$6.3 \cdot 10^{-4}$
313.2		$1.07 \cdot 10^{-3}$ (T; Ref. 11)	$1.1 \cdot 10^{-3}$
374.2	124 (Ref. 4)	$8.42 \cdot 10^{-3}$ (T; Ref. 4)	$8.4 \cdot 10^{-3}$
423.2	520 (Ref. 10)	$2.80 \cdot 10^{-2}$ (T; Ref. 10)	$3.1 \cdot 10^{-2}$
424.7	531 (Ref. 4)	$3.76 \cdot 10^{-2}$ (T; Ref. 4)	$3.2 \cdot 10^{-2}$
473.2	1790 (Ref. 10)	$9.50 \cdot 10^{-2}$ (T; Ref. 10)	$9.4 \cdot 10^{-2}$
475.2	1779 (Ref. 4)	$1.18 \cdot 10^{-1}$ (T; Ref. 4)	$9.8 \cdot 10^{-2}$
498.2	2900 (Ref. 10)	$1.62 \cdot 10^{-1}$ (T; Ref. 10)	$1.6 \cdot 10^{-1}$
523.2	4630 (Ref. 10)	$2.48 \cdot 10^{-1}$ (T; Ref. 10)	$2.6 \cdot 10^{-1}$
548.2	7180 (Ref. 10)	$4.03 \cdot 10^{-1}$ (T; Ref. 10)	$4.2 \cdot 10^{-1}$
558.2	8230 (Ref. 10)	$5.04 \cdot 10^{-1}$ (T; Ref. 10)	$5.1 \cdot 10^{-1}$
563.2	9360 (Ref. 10)	$6.06 \cdot 10^{-1}$ (T; Ref. 10)	$5.7 \cdot 10^{-1}$
576.2	11 238 (Ref. 4)	$5.95 \cdot 10^{-1}$ (T; Ref. 4)	$8.1 \cdot 10^{-1}$

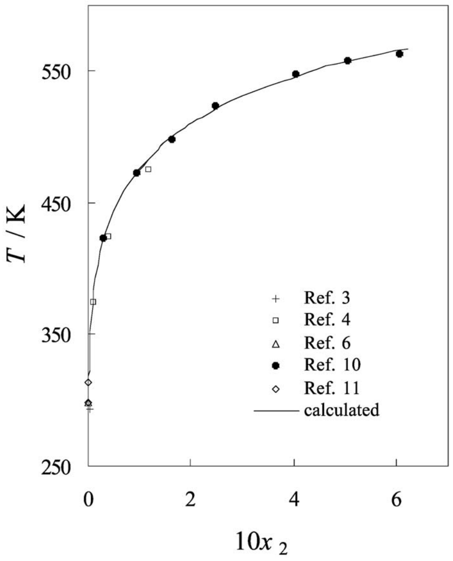

FIG. 9. All the solubility data for water (2) in decane (1).

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Prepr. **3**, C-61 (1958).

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of decane-1-C^{14} in water at 25 °C was reported to be $16 \cdot 10^{-9}$ g (1)/g (2). The corresponding mole fraction, calculated by the compiler, is $x_1 = 2.0 \cdot 10^{-9}$.

Auxiliary Information

Method/Apparatus/Procedure:

Carbon-14 labeled (1) was used as radioactive tracer. The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)–(2) dispersion has been described in Baker.[1] A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).

Source and Purity of Materials:

(1) Nuclear Instrument and Chemical Corporation; used as received.
(2) Distilled.

Estimated Error:

Solubility: 20% (standard deviation from 17 replicate runs).

References:

[1] E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Reprints-Symposia, **1**, No. 2, 5 (1956).

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. G. Baker, Science **129**, 871 (1959).

Variables:

One temperature: 25 °C

Prepared By:

F. Kapuku

Experimental Values

The solubility of decane in water at 25 °C was reported to be $22 \cdot 10^{-7}$ mL (1)/100 mL (2).
The corresponding mole fraction, calculated by the compiler, is $x_1 = 2.0 \cdot 10^{-9}$.

Auxiliary Information

Method/Apparatus/Procedure:

Not specified.

Source and Purity of Materials:

Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	A. Becke and G. Quitzsch, Chem. Tech. (Leipzig) **29**, 49 (1977).
Variables:	**Prepared By:**
One temperature: 20 °C	P. L. Huyskens and M. C. Haulait-Pirson

Experimental Values

The solubility of decane in water at 20 °C was reported to be in mole fraction, $x_1 = 2.5 \cdot 10^{-9}$. The corresponding mass percent, calculated by the compiler, is $1.976 \cdot 10^{-6}$ g (1)/100 g sln.

The solubility of water in decane at 20 °C was reported to be in mole fraction, $x_2 = 2.3 \cdot 10^{-3}$. The corresponding mass percent, calculated by the compiler, is 0.0292 g (2)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

The refractometric and the Karl Fischer dead-stop titration methods were used. No more details are given in the paper.

Source and Purity of Materials:

Not specified.

Estimated Error:

Solubility: 0.05%–1% for (1) in (2); 0.3%–1.3% for (2) in (1).

Components:	**Original Measurements:**
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
Variables:	**Prepared By:**
Temperature: 374.15–576.15 K Pressure: 0.124–11.238 MPa	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of decane in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^5 \cdot x_1$
374.15	0.124	0.000095	0.012
424.65	0.531	0.000261	0.033
475.15	1.779	0.00111	0.14
576.15[a]	11.238	0.0387	4.9

Solubility of water in decane

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
374.15	0.124	0.1074	0.00842
424.65	0.531	0.492	0.0376
475.15	1.779	1.67	0.118
576.15[a]	11.238	15.68	0.595
566.71[b]	9.639	23.32	0.706

[a] Above three-phase critical end point.

[b] Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of (1) in (2) was measured by glc, while that of (2) in (1) by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus.

Source and Purity of Materials:

(1) Philips; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:

Temperature: ±0.6 K at critical end point.[b]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[b]
Pressure: 1% and ±0.04 MPa at critical end point.[b]

References:

[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

Components:	**Original Measurements:**
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	F. Franks, Nature (London) **210**, 87 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	F. Kapuku

Experimental Values

The solubility of decane in water at 25 °C was reported to be, in mole fraction, $x_1 = 2.5 \cdot 10^{-9}$.

The corresponding mass percent calculated by the compiler is $1.98 \cdot 10^{-6}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

The analysis was performed by glc. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator column, and (2) was removed by Drierite. The (1) concentrations were obtained from the peak areas, after initial calibrations.

Source and Purity of Materials:

(1) Fluka; purum grade; purity>97% (chromatographic analysis).
(2) Not specified.

Estimated Error:

Solubility: ±12%.

Components:	**Original Measurements:**
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	S. Hellinger and S. I. Sandler, J. Chem. Eng. Data **40**, 321 (1995).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of decane in water

$t/°C$	$10^6 \cdot$ g (1)/100 g sln (compilers)	$10^9 \cdot x_1$
25.0	4.95	6.27
	4.84	6.13

Solubility of water in decane

$t/°C$	$10^3 \cdot$ g (2)/100 g sln (compilers)	$10^4 \cdot x_2$
25.0	6.8	5.4
	6.6	5.2

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. An equilibrium cell, thermostatically jacketed to maintain temperature to within ±0.1 °C, was described in Magnussen *et al.*[1] Samples of the both phases were withdrawn using a Perfectum Model MicroMate hypodermic syringe. Analysis of (1) in (2) was done using a Hewlett-Packard Model 5730 gas chromatograph with thermal conductivity detector and a Poropak Q column. For determination of (2) in (1) Karl Fischer titration, McAuliffe,[2] was used. Every sample was analyzed three times.

Source and Purity of Materials:

(1) Aldrich Chemical Co.; purity >99%; used as received.
(2) De-ionized with Barnstead NANO pure equipment.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±2%.

References:

[1] T. Magnussen, P. Rasmussen, and Aa. Fredenslund, Ind. Eng. Chem. Process Des. Dev. **20**, 331 (1981).
[2] C. McAuliffe, Nature (London) **200**, 1002 (1963).

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski

Experimental Values

The solubility of decane in water at 25 °C was reported to be $x_1 = 1.1 \cdot 10^{-9}$.

The corresponding mass percent calculated by the compiler is $8.7 \cdot 10^{-7}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigouously stirred magnetically for 10–12 h. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20 mL aliquots were introduced into 40 mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1) saturated air was analyzed by glc.

Source and Purity of Materials:

(1) Source not specified; CP reagent; purity not specified.
(2) Distilled.

Estimated Error:

Not specified.

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. **573**, 251 (1975).

Variables:

Not specified.

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The authors reported two different values for the solubility of decane in water: 0.182 and 1.22 mg (1)/L sln.

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percents calculated by the compiler are 0.0000182 and 0.000122 g (1)/100 g sln and the corresponding mole fractions, x_1 , are $2.3 \cdot 10^{-8}$ and $1.6 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibrations it is possible to calculate the amount of (1) in the original sample.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not estimated.

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. McAuliffe, Science **163**, 478 (1969).

Variables:

One temperature: 25 °C

Prepared By:

F. Kapuku

Experimental Values

The solubility of decane in water at 25 °C was reported to be 0.052 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $5.2 \cdot 10^{-6}$ g (1)/100 g sln and $6.58 \cdot 10^{-9}$.

Auxiliary Information

Method/Apparatus/Procedure:

(1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 min. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.

Source and Purity of Materials:

(1) Not specified.
(2) Distilled.

Estimated Error:

Solubility: ±0.0043 mg (1)/kg (2).

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Yu. Namiot, V. G. Skripka, and Yu. G. Lotter, Zh. Fiz. Khim. **50**, 2718 (1976); 2718 Deposited doc. VINITI 1213-76.

Variables:

Temperature: 150–310 °C
Pressure: 0.52–8.44 MPa

Prepared By:

A. Maczynski

Experimental Values

Solubility of water in decane

t/°C	x_2	g (2)/100 g sln (compiler)	P/kg·cm^{-2}	P/MPa (compiler)
150	0.028	0.36	5.3	0.52
200	0.095	1.31	18.2	1.79
225	0.162	2.39	30	2.9
250	0.248	4.01	47.2	4.63
275	0.403	7.87	73.2	7.18
285	0.504	11.4	83.9	8.23
290	0.606	16.3	95.4	9.36
310	0.029	0.38	20	2.0
310	0.069	0.93	30	2.9
310	0.114	1.60	40	3.0
310	0.171	2.54	50	4.9
310	0.239	3.82	60	5.9
310	0.313	5.45	70	6.9
310	0.407	7.99	80	7.8
310	0.520	12.06	86.1	8.44

Auxiliary Information

Method/Apparatus/Procedure:

The static method for vapor–liquid equilibrium described in Sultanov *et al.*[1] was used. No more details were reported in the paper.

Source and Purity of Materials:

(1) Source not specified; CP reagent; used as received.
(2) Distilled.

Estimated Error:

Not specified.

References:

[1] R. G. Sultanov, V. E. Skripka, and Yu. A. Namiot, Zh. Fiz. Khim. **46**, 2170 (1976).

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).

Variables:

Temperature: 25 and 40 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

Solubility of water in decane

$t/°C$	$10^4 \cdot x_2$	mg (2)/kg sln
25	5.7	72[a]
40	10.7	136[b]

[a,b]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water bath for 7 days. A 20 mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0–1.3 mg (2)/mL was used to titrate (2) in (1) directly in the presence on methanol to a dead-stop end-point using a Beckman KF3 automatic titrimeter.

Source and Purity of Materials:

(2) Distilled and de-ionized.

Estimated Error:

Solubility: (a) 0%–6%; (b) 0%–2% (deviations from the mean).

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skripka, Tr. Vses. Neftegazov. Nauch. Issled. Inst. **61**, 139 (1976).

R. G. Sultanov and V. E. Skripka, Zh. Fiz. Khim. **47**, 1035 (1973).

Variables:

Temperature: 228–290 °C
Pressure: 2.9–78.5 MPa

Prepared By:

A. Maczynski

Experimental Values

Solubility of water in decane

$t/°C$	x_2	g (2)/100 g sln (compiler)	$P/\text{kg}\cdot\text{cm}^{-2}$	P/MPa (compiler)
225	0.162	2.39	30	2.9
	0.157	2.30	50	4.9
	0.153	2.28	70	6.9
	0.148	2.15	100	9.8
	0.138	1.99	150	14.7
	0.132	1.89	200	19.6
	0.124	1.76	250	24.5
	0.118	1.67	300	29.4
	0.108	1.51	400	39.2
	0.102	1.42	500	49.0
	0.098	1.36	600	58.8
	0.095	1.31	700	68.6
	0.094	1.30	800	78.5
250	0.255	4.15	50	4.9
	0.248	4.01	70	6.9
	0.240	3.84	100	9.8
	0.226	3.56	150	14.7
	0.213	3.31	200	19.6
	0.200	3.07	250	24.5
	0.190	2.88	300	29.4
	0.168	2.49	400	39.2
	0.158	2.32	500	49.0
	0.153	2.24	600	58.8
	0.151	2.20	700	68.6
	0.148	2.15	800	78.5
275	0.404	7.90	70	6.9
	0.385	7.34	100	9.8
	0.353	6.46	150	14.7
	0.320	5.62	200	19.6
	0.293	4.98	250	24.5
	0.272	4.52	300	29.4
	0.246	3.97	400	39.2
	0.231	3.66	500	49.0
	0.217	3.39	600	58.8
	0.204	3.14	700	68.6
	0.197	3.08	800	78.5
290	0.580	14.88	100	9.8
	0.417	8.30	150	14.7
	0.392	7.54	200	19.6
	0.371	6.95	250	24.5

0.350	6.38	300	29.4
0.318	5.57	400	39.2
0.291	4.94	500	49.0
0.270	4.47	600	58.8
0.253	4.11	700	68.6
0.243	3.90	800	78.5

Auxiliary Information

Method/Apparatus/Procedure:

The experimental technique was described in Sultanov *et al.*[1] No details reported in the paper.

Source and Purity of Materials:

(1) Source not specified, chemical reagent grade; purity not specified; used as received.
(2) Distilled.

Estimated Error:

Not specified.

References:

[1] R. G. Sultanov, V. E. Skripka, and A. Yu. Namiot, Gazov. Prom. **4**, 6 (1971).

Components:

(1) Decane; $C_{10}H_{22}$; [124-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Q. Wang and K.-C. Chao, Fluid Phase Equilib. **59**, 207 (1990).

Variables:

Temperature: 573.2– 613.2 K
Pressure: 92.0–231.0 bar

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazei

Experimental Values

Solubility of decane in water

T/K	P/bar	g (1)/100 g sln (compilers)	x_1
573.2	92.0	26.52	0.0437
	100.0	55.96	0.1386
	104.5	64.02	0.1839
	109.0	69.35	0.2227
	121.0	78.60	0.3174
	130.5	82.91	0.3805
	144.0	85.37	0.4249
	161.0	87.84	0.4777
	178.5	89.09	0.5083
	198.5	89.33	0.5146
593.2	121.7	29.06	0.0493
	130.5	49.09	0.1088
	136.0	57.72	0.1474
	151.1	70.81	0.3350
	171.5	78.84	0.3206
	186.2	81.31	0.3552
	201.0	82.97	0.3816
613.2	150.2	5.99	0.0080
	160.0	24.37	0.0392
	163.5	29.23	0.0497
	178.5	47.75	0.1037
	190.0	56.51	0.1413
	202.0	62.31	0.1731
	231.0	69.00	0.2199

Solubility of water in decane

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
573.2	92.0	100.00	1.0000
	100.0	100.00	1.0000
	104.5	100.00	1.0000
	109.0	100.00	1.0000
	121.0	100.00	1.0000
	130.5	100.00	1.0000
	144.0	100.00	1.0000
	161.0	99.61	0.9995
	178.5	97.68	0.9970
	198.5	96.18	0.9950
593.2	121.7	100.00	1.0000
	130.5	100.00	1.0000
	136.0	100.00	1.0000

	151.1	100.00	1.0000
	171.5	98.06	0.9975
	186.2	97.53	0.9968
	201.0	97.15	0.9963
613.2	150.2	100.00	1.0000
	160.0	100.00	1.0000
	163.5	98.21	0.9977
	178.5	97.00	0.9961
	190.0	97.14	0.9962
	202.0	97.15	0.9963
	231.0	97.00	0.9961

Auxiliary Information

Method/Apparatus/Procedure:

Flow apparatus for the high temperature experiments was used. Streams of both components were combined, mixed, preheated, and pumped into a stainless equilibrium cell of 10 mL volume with two transparent sapphire windows. Pressure was measured with a Heise Bourdon-tube gauge. Details of the apparatus and procedure were described in the paper. Both phases were sampled, cooled, homogenized with 1-propanol, and analyzed by glc (Hewlett Packard 5710 A, 2 m column packed with Chromosorb 102, thermal conductivity detector, intergrator Hewlett Packard 21MX).

Source and Purity of Materials:

(1) Wako Pure Chem. Ind.; purity >99.5 mole % by glc; used as received.
(2) Distilled water was purified by Milliq-Labo (Millipore Co.) equipment.

Estimated Error:

Solubility: ±0.001 mole fraction.
Temperature: <±0.1 K.
Pressure: ±0.5 bar.

2.20. 2,7-Dimethyloctane+Water

Components:

(1) 2,7-Dimethyloctane; $C_{10}H_{22}$; [1072-16-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:

Temperature: 10–30 °C

Prepared By:

A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in 2,7-dimethyloctane

t/°C	$10^4 \cdot x_2$ (compiler)	G (2)/100 g sln
10	3.79	0.0048
20	6.87	0.0087
30	12.00	0.0152

Auxiliary Information

Method/Apparatus/Procedure:

Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

3. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

4. Registry Number Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

5. Author Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

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