IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 8. C_9 Hydrocarbons with Water

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The mutual solubility and related liquid-liquid equilibria of C_9 hydrocarbons with water are exhaustively and critically reviewed. Reports of the experimental determination of solubility in 18 chemically distinct binary systems that appeared in the primary literature prior to the end of 2002 are compiled. For 8 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 Date 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. © *2005 American Institute of Physics.* [DOI: 10.1063/1.1842098]

Key words: C_9 hydrocarbons; critical evaluation; liquid-liquid equilibria; solubility; water.

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1. Preface

1.1. Scope of this Volume

This paper is Part 8 of a revised and updated version of an earlier compilation and evaluation of the mutual solubility of

water and hydrocarbon compounds containing five or more carbon atoms (Shaw[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 (Ref. 7). The derivation of the smoothing equations used for calculate reference values can be found in Parts 1 and 2 (Refs. 7 and 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 C_5 to C_7* (Pergamon, New York, 1989).
[2] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 38, *Hydrocarbons with Water and Seawater, Part II: Hydrocarbons* C_8 to C_{36} (Pergamon, New York, 1989).
[3] A. Maczynski, M. Goral, B. Wisniewska-Goclowska, A. Skrzecz, and D. Shaw, Monatshefte Chemie **134**, 633 (2003).
[4] A. Maczynski, B. Wisniewska-Goclowska, and M. Goral, *Recommended Liquid-Liquid Equilibrium Data. Part 1. Binary Alkane-Water Systems*, J. Phys. Chem. Ref. Data **33**, 549 (2004).
[5] M. Goral, B. Wisniewska-Goclowska, and A. Maczynski, *Recommended Liquid-Liquid Equilibrium Data. Part 2. Unsaturated Hydrocarbon-Water Systems*, J. Phys. Chem. Ref. Data **33**, 579 (2004).
[6] B. Wisniewska-Goclowska, M. Goral, and A. Maczynski, *Recommended Liquid-Liquid Equilibrium Data. Part 3. Binary Aromatic Hydrocarbon-Water Systems*, J. Phys. Chem. Ref. Data **33**, 1159 (2004).
[7] A. Maczynski and D. Shaw, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocharbons with Water and Seawater-Revised and Updated. Part 1. C_5 Hydrocarbons with Water*, J. Phys. Chem. Ref. Data **34**, 441 (2005).
[8] A. Maczynski and D. Shaw, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater-Revised and Updated. Part 2. Benzene with Water and Heavy Water*, J. Phys. Chem. Ref. Data **34**, 477 (2005).

2. C_9 Hydrocarbons with Water

2.1. Indan+Water

Components:
(1) Indan; C_9H_{10}; [496-11-7]
(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 Data

The solubility of indan in water at 25 °C and at system pressure was reported to be 88.9 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00889 $g(1)$/100 g sln and $1.35 \cdot 10^{-5}$.

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: ±2.7 mg(1)/kg(2).

Components:
(1) Indan; C_9H_{10}; [496-11-7]
(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 Data

The solubility of indan in water at 25 °C was reported to be: 109.1 mg (1)/L sln and $x_1 = 1.665 \cdot 10^{-5}$.

The corresponding mass percent calculated by the compiler is 0.01091 $g(1)$/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: ±1.02 mg(1)/L sln (maximum deviation from several determinations).

2.2. 1-Ethyl-2-methylbenzene+Water

Components:
(1) 1-Ethyl-2-methylbenzene; C_9H_{12} ; [611-14-3]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of 1-ethyl-2-methylbenzene in water

t/°C	mol (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
25.0	$6.21 \cdot 10^{-4}$	$7.49 \cdot 10^{-3}$	$1.122 \cdot 10^{-5}$

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 (2) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by hplc. 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).

2.3. Isopropylbenzene (cumene)+Water*

Components:
(1) Isopropylbenzene (cumene); C_9H_{12} ; [98-82-8]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Isopropylbenzene (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
Andrews and Keefer[1]	298	Price[6]	298
Glew and Robertson[3]	298–353	Sanemasa *et al.*[7]	288–318
McAuliffe[4]	298	Stearns *et al.*[8]	298
McAuliffe[5]	298	Sutton and Calder[9]	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:

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

where $\ln x_{\min,1} = -11.53$, $D = 45.78$, and $T_{\min} = 290$.

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 listed in Table 1.

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

TABLE 1. The data categories for solubility of isopropylbenzene (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]
288.2		Sanemasa *et al.*[7]	
298.1		Glew and Robertson[3]	
298.2	Andrews and Keefer[1]	McAuliffe[4]	Stearns *et al.*[8]
	Sutton and Calder[9]	McAuliffe[5]	
	Sanemasa *et al.*[7]	Price[6]	
303.1		Glew and Robertson[3]	
308.1		Glew and Robertson[3]	
308.2		Sanemasa *et al.*[7]	
313.1		Glew and Robertson[3]	
318.1		Glew and Robertson[3]	
318.2		Sanemasa *et al.*[7]	
323.1		Glew and Robertson[3]	
328.1		Glew and Robertson[3]	
333.1		Glew and Robertson[3]	
338.3		Glew and Robertson[3]	
343.5		Glew and Robertson[3]	
348.3		Glew and Robertson[3]	
353.4		Glew and Robertson[3]	

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

T/K	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
288.2	$8.92 \cdot 10^{-6}$ (T; Ref. 7)	$9.9 \cdot 10^{-6}$
298.1	$1.20 \cdot 10^{-5}$ (T; Ref. 3)	$1.0 \cdot 10^{-5}$
298.2	$1.09 \cdot 10^{-5}$ (R; Ref. 1), $7.90 \cdot 10^{-6}$ (T; Ref. 4), $7.50 \cdot 10^{-6}$ (T; Ref. 5), $7.23 \cdot 10^{-6}$ (T; Ref. 6), $9.22 \cdot 10^{-6}$ (R; Ref. 7), $2.50 \cdot 10^{-5}$ (D; Ref. 8), $9.78 \cdot 10^{-6}$ (R; Ref. 9)	$1.0 \cdot 10^{-5}$
303.1	$1.24 \cdot 10^{-5}$ (T; Ref. 3)	$1.0 \cdot 10^{-5}$
308.1	$1.28 \cdot 10^{-5}$ (T; Ref. 3)	$1.1 \cdot 10^{-5}$
308.2	$1.03 \cdot 10^{-5}$ (T; Ref. 7)	$1.1 \cdot 10^{-5}$
313.1	$1.34 \cdot 10^{-5}$ (T; Ref. 3)	$1.1 \cdot 10^{-5}$
318.1	$1.42 \cdot 10^{-5}$ (T; Ref. 3)	$1.2 \cdot 10^{-5}$
318.2	$1.16 \cdot 10^{-5}$ (T; Ref. 7)	$1.2 \cdot 10^{-5}$
323.1	$1.50 \cdot 10^{-5}$ (T; Ref. 3)	$1.3 \cdot 10^{-5}$
328.1	$1.60 \cdot 10^{-5}$ (T; Ref. 3)	$1.4 \cdot 10^{-5}$
333.1	$1.72 \cdot 10^{-5}$ (T; Ref. 3)	$1.5 \cdot 10^{-5}$
338.3	$1.86 \cdot 10^{-5}$ (T; Ref. 3)	$1.6 \cdot 10^{-5}$
343.5	$2.03 \cdot 10^{-5}$ (T; Ref. 3)	$1.8 \cdot 10^{-5}$
348.3	$2.21 \cdot 10^{-5}$ (T; Ref. 3)	$2.0 \cdot 10^{-5}$
353.4	$2.42 \cdot 10^{-5}$ (T; Ref. 3)	$2.2 \cdot 10^{-5}$

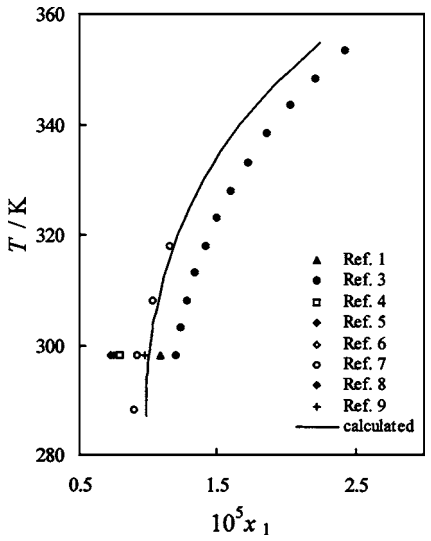

Fig. 1. All the solubility data for isopropylbenzene (1) in water (2).

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

The experimental solubility data for (2) in (1) have been investigated by Englin *et al.*[2] at 273–323 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:

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

where $d_1 = -0.329$, $d_2 = -2.962$, $d_3 = 0.152$, $d_4 = -6.247$, and $T_r = T/574.0$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of isopropylbenzene 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 categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 3 and shown in Fig. 2. Since only one experimental data point is available at each temperature, no data can be Recommended. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

TABLE 3. Experimental values for solubility of water (2) in isopropylbenzene (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
273.2	$1.04 \cdot 10^{-3}$ (T; Ref. 2)	$1.2 \cdot 10^{-3}$
283.2	$1.46 \cdot 10^{-3}$ (T; Ref. 2)	$1.6 \cdot 10^{-3}$
293.2	$2.02 \cdot 10^{-3}$ (T; Ref. 2)	$2.2 \cdot 10^{-3}$
303.2	$2.71 \cdot 10^{-3}$ (T; Ref. 2)	$3.0 \cdot 10^{-3}$
313.2	$3.66 \cdot 10^{-3}$ (T; Ref. 2)	$4.0 \cdot 10^{-3}$
323.2	$4.72 \cdot 10^{-3}$ (T; Ref. 2)	$5.3 \cdot 10^{-3}$

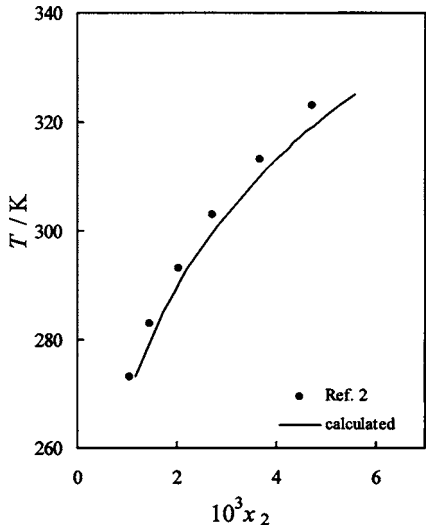

Fig. 2. All the solubility data for water (2) in isopropylbenzene (1).

Rejected Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[10] 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]D. N. Glew and R. E. Robertson, J. Phys. Chem. **60**, 332 (1956).
[4]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[5]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[6]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[7]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[8]R. S. Stearns, H. Oppenheimer, E. Simon, and W. D. Harkins, J. Chem. Phys. **15**, 496 (1947).
[9]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[10]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Components:	**Original Measurements:**
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8] (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 Data

The solubility of isopropylbenzene in water at 25 °C was reported to be 0.0073 $g(1)$/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $1.09 \cdot 10^{-5}$.

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. white label; fractionally distilled; boiling point range 151.5 °C–152.0 °C.
(2) Not specified.

Estimated Error: Not specified.

Components:
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8]
(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: 0 °C–50 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in isopropylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
0	1.04	0.0156
10	1.46	0.0219
20	2.02	0.0303
30	2.71	0.0407
40	3.66	0.0550
50	4.72	0.0710

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostated 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) Isopropylbenzene; C_9H_{12} ; [98-82-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. N. Glew and R. E. Robertson, J. Phys. Chem. **60**, 332 (1956).

Variables:
Temperature: 298 K–353 K

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of isopropylbenzene in water

T/K	$10^5 \cdot x_1$	$g(1)$/100 g sln (compiler)
298.086	1.2050	0.00804
303.134	1.2416	0.00829
308.068	1.2825	0.00856
313.108	1.3446	0.00897
318.055	1.4162	0.00945
323.052	1.5037	0.01004
328.066	1.6011	0.01069
333.133	1.7221	0.01149
338.315	1.8624	0.01243
343.470	2.0302	0.01355
348.247	2.2064	0.01472
353.359	2.4212	0.01616

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was floated on the surface of the main body of the water and the aqueous solution was pumped steadily in a closed circuit through a quartz absorption cell where its absorbance was measured. From these values the solubility of (1) in (2) was calculated.

Source and Purity of Materials:
(1) Eastman Kodak Co. White Label; distilled in an atmosphere of nitrogen; boiling point range 0.2 °C, passed repeatedly through a fresh column of Fisher activated alumina.
(2) Distilled; passed through a demineralizing column.

Estimated Error:
Temperature: ±0.002 K.
Solubility: ±1.00% at 25 °C and ±1.25% at 80 °C (standard error).

Components:	Original Measurements:
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, Nature (London) **200**, 1092 (1963).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of isopropylbenzene in water at 25 °C was reported to be $0.0053g(1)$/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $7.9 \cdot 10^6$.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was prepared by either shaking vigourously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; 99+%; used as received.
(2) Distilled.

Estimated Error:

Temperature: ± 1.5 °C.
Solubility: 0.0005 (standard deviation of mean).

Components:	Original Measurements:
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of isopropylbenzene in water at 25 °C was reported to be 50 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are $0.0050g(1)$/100 g sln and $7.5 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250 mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjuction with a flame ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ± 1.5 °C.
Solubility: 5 mg (1)/kg (2) (std. dev. of mean).

Components:
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of isopropylbenzene in water

t/°C	$10^6 \cdot x_1$ (compiler)[a]	$10^3 \cdot g(1)/100$ g sln (compiler)[a]	$10^4 \cdot$ mol(1)/L sln
15	8.92	5.95	4.95±0.28
25	9.22	6.15	5.10±0.45
35	10.3	6.87	5.68±0.22
45	11.6	7.75	6.38±0.24

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostated flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8]
(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 Data

The solubility of isopropylbenzene in water at 25 °C and at system pressure was reported to be 48.3 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $0.00483 g(1)/100$ g sln and $7.23 \cdot 10^{-6}$.

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: ±1.2 mg(1)/kg(2).

Components:	Original Measurements:
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8] (2) Water; H_2O; [7732-18-5]	R. S. Stearns, H. Oppenheimer, E. Simon, and W. D. Harkins, J. Chem. Phys. **15**, 496 (1947).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and D. Shaw

Experimental Data

The solubility of isopropylbenzene in water at 25 °C was reported to be $0.017g(1)/100$ g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $2.5 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

Mixtures of (1) in (2) of known composition were shaken for at least 48 h. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±3 °C.

Components:	Original Measurements:
(1) Isopropylbenzene; C_9H_{12} ; [98-82-8] (2) Water; H_2O; [7732-18-5]	C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of isopropylbenzene in water at 25 °C was reported to be 65.3 mg (1)/kg (2).

The corresponding mass percent and the mole fraction, x_1, calculated by the compilers are $0.00653g(1)/100$ g sln and $9.78 \cdot 10^{-6}$.

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: 0.8 (standard deviation of the mean for six replicates).

2.4. 1,8-Nonadiyne+Water

Components:
(1) 1,8-Nonadiyne; C_9H_{12} ; [2396-65-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

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

Experimental Data

The solubility of 1,8-nonadiyne in water at 25 °C was reported to be 125 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are $0.0125g(1)/100$ g sln and $1.9\cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjuction with a flame ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: mp. ±1.5 °C.
Solubility: 3 mg (1)/kg (2) (standard deviation of mean).

2.5. Propylbenzene+Water*

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

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

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

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

Author (s)	T/K	Author (s)	T/K
Andrews and Keefer[1]	298	Sanemasa *et al.*[9]	298
Dohanyosova *et al.*[2]	274–328	Sanemasa *et al.*[10]	298
Führer[3]	288	Sawamura *et al.*[11]	298
Guseva and Parnov[4]	359–495	Sawamura *et al.*[12]	273–323
Klevens[5]	298	Stearns *et al.*[13]	298
Krasnoshchekova and Gubergrits[6]	298	Tewari *et al.*[14]	298
Owens *et al.*[7]	283–318	DeVoe *et al.*[15]	288–303
Sanemasa *et al.*[8]	288–318		

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:

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

where $\ln x_{\min,1} = -11.65$, $D = 46.32$, and $T_{\min} = 290$.

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 listed in Table 4.

All the experimental and reference data are listed in Table 5 and shown in Fig. 3. The recommended and tentative data are shown in Fig. 4.

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

The experimental high pressure solubility for (1) in (2) investigated by Sawamura *et al.*[12] at 298 K–323 K and 25 000 kPa–400 000 kPa have not been critically evaluated because the developed method is not applied for such data.

Rejected and Inaccessible Data

The data reported by Alwani and Schneider[16] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[2]P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001).
[3]H. Führer, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).
[4]A. N. Guseva and E. I. Parnov, Zh. Fiz. Khim. **38**, 805 (1964).
[5]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[6]R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy **2**, 170 (1975).
[7]J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).
[8]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[9]I. Sanemasa, S. Arakawa, M. Araki, and T. Deguchi, Bull. Chem. Soc. Jpn. **57**, 1539 (1984).
[10]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).
[11]S. Sawamura, K. Kitamura, and Y. Taniguchi, J. Phys. Chem. **93**, 4931 (1989).
[12]S. Sawamura, K. Nagaoka, and T. Machikawa, J. Phys. Chem. **105**, 2429 (2001).
[13]R. S. Stearns, H. Oppenheimer, E. Simon, and W. D. Harkins, J. Chem. Phys. **15**, 496 (1947).
[14]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[15]H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (U.S.) **86**, 361 (1981).
[16]Z. Alwani and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **73**, 294 (1969).

TABLE 4. The data categories for solubility of propylbenzene (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		Sawamura *et al.*[12]	
273.7		Dohanyosova *et al.*[2]	
278.2		Dohanyosova *et al.*[2]	
		Sawamura *et al.*[12]	
283.2	Owens *et al.*[7]		
	Sawamura *et al.*[12]		
288.2	Führer[3]	Dohanyosova *et al.*[2]	
	Sawamura *et al.*[12]	Owens *et al.*[7]	
		Sanemasa *et al.*[8]	
		DeVoe *et al.*[15]	
293.2	Owens *et al.*[7]	DeVoe *et al.*[15]	
	Sawamura *et al.*[12]		
298.1		Sanemasa *et al.*[10]	
298.2	Andrews and Keefer[1]	Dohanyosova *et al.*[2]	Klevens[5]
	Owens *et al.*[7]	Krasnoshchekova and	Sawamura *et al.*[11]
	Sawamura *et al.*[12]	Gubergrits[6]	Stearns *et al.*[13]
		Sanemasa *et al.*[8]	
		Sanemasa *et al.*[9]	
		Tewari *et al.*[14]	
		DeVoe *et al.*[15]	
303.2	Owens *et al.*[7]		
	Sawamura *et al.*[12]		
	DeVoe *et al.*[15]		
308.2	Owens *et al.*[7]	Dohanyosova *et al.*[2]	
	Sanemasa *et al.*[8]		
	Sawamura *et al.*[12]		
313.2	Owens *et al.*[7]		
	Sawamura *et al.*[12]		
318.2	Dohanyosova *et al.*[2]		
	Owens *et al.*[7]		
	Sanemasa *et al.*[8]		
	Sawamura *et al.*[12]		
323.2		Sawamura *et al.*[12]	
328.2		Dohanyosova *et al.*[2]	
359.0		Guseva and Parnov[4]	
387.7			Guseva and Parnov[4]
413.7			Guseva and Parnov[4]
461.2			Guseva and Parnov[4]
495.2			Guseva and Parnov[4]

TABLE 5. Experimental values for solubility of propylbenzene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$9.01 \cdot 10^{-6}$ (T; Ref. 12)	$9.5 \cdot 10^{-6}$
273.7	$6.98 \cdot 10^{-6}$ (T; Ref. 2)	$9.4 \cdot 10^{-6}$
278.2	$6.86 \cdot 10^{-6}$ (T; Ref. 2), $8.65 \cdot 10^{-6}$ (T; Ref. 12)	$9.1 \cdot 10^{-6}$
283.2	$8.06 \cdot 10^{-6}$ (R; Ref. 7), $8.38 \cdot 10^{-6}$ (R; Ref. 12)	$8.8 \cdot 10^{-6}$
288.2	$6.73 \cdot 10^{-6}$ (T; Ref. 2), $9.00 \cdot 10^{-6}$ (R; Ref. 3), $7.84 \cdot 10^{-6}$ (T; Ref. 7), $6.99 \cdot 10^{-6}$ (T; Ref. 8), $8.23 \cdot 10^{-6}$ (R; Ref. 12), $7.68 \cdot 10^{-6}$ (T; Ref. 15)	$8.7 \cdot 10^{-6}$
293.2	$8.16 \cdot 10^{-6}$ (R; Ref. 7), $8.16 \cdot 10^{-6}$ (R; Ref. 12), $7.67 \cdot 10^{-6}$ (T; Ref. 15)	$8.7 \cdot 10^{-6}$
298.1	$7.50 \cdot 10^{-6}$ (T; Ref. 10)	$8.9 \cdot 10^{-6}$
298.2	$8.20 \cdot 10^{-6}$ (R; Ref. 1), $7.24 \cdot 10^{-6}$ (T; Ref. 2), $1.80 \cdot 10^{-5}$ (D; Ref. 5), $1.05 \cdot 10^{-5}$ (T; Ref. 6), $8.00 \cdot 10^{-6}$ (R; Ref. 7), $7.64 \cdot 10^{-6}$ (T; Ref. 8), $6.78 \cdot 10^{-6}$ (T; Ref. 9), $1.39 \cdot 10^{-5}$ (D; Ref. 11), $8.23 \cdot 10^{-6}$ (R; Ref. 12), $1.80 \cdot 10^{-5}$ (D; Ref. 13), $7.84 \cdot 10^{-6}$ (T; Ref. 14), $7.80 \cdot 10^{-6}$ (T; Ref. 15)	$8.9 \cdot 10^{-6}$
303.2	$7.91 \cdot 10^{-6}$ (R; Ref. 7), $8.41 \cdot 10^{-6}$ (R; Ref. 12), $8.05 \cdot 10^{-6}$ (R; Ref. 15)	$9.1 \cdot 10^{-6}$
308.2	$7.86 \cdot 10^{-6}$ (T; Ref. 2), $8.54 \cdot 10^{-6}$ (R; Ref. 7), $8.25 \cdot 10^{-6}$ (R; Ref. 8), $8.74 \cdot 10^{-6}$ (R; Ref. 12)	$9.4 \cdot 10^{-6}$
313.2	$9.66 \cdot 10^{-6}$ (R; Ref. 7), $9.18 \cdot 10^{-6}$ (R; Ref. 12)	$9.9 \cdot 10^{-6}$
318.2	$9.46 \cdot 10^{-6}$ R; (Ref. 2), $1.01 \cdot 10^{-5}$ (R; Ref. 7), $9.61 \cdot 10^{-6}$ (R; Ref. 8), $9.82 \cdot 10^{-6}$ (R; Ref. 12)	$1.1 \cdot 10^{-5}$
323.2	$1.06 \cdot 10^{-5}$ (T; Ref. 12)	$1.1 \cdot 10^{-5}$
328.2	$1.13 \cdot 10^{-5}$ (T; Ref. 2)	$1.2 \cdot 10^{-5}$
359.0	$1.98 \cdot 10^{-5}$ (T; Ref. 4)	$2.2 \cdot 10^{-5}$
387.7	$2.49 \cdot 10^{-5}$ (D; Ref. 4)	$4.4 \cdot 10^{-5}$
413.7	$4.81 \cdot 10^{-5}$ (D; Ref. 4)	$8.8 \cdot 10^{-5}$
461.2	$1.30 \cdot 10^{-4}$ (D; Ref. 4)	$3.5 \cdot 10^{-4}$
495.2	$3.68 \cdot 10^{-4}$ (D; Ref. 4)	$9.4 \cdot 10^{-4}$

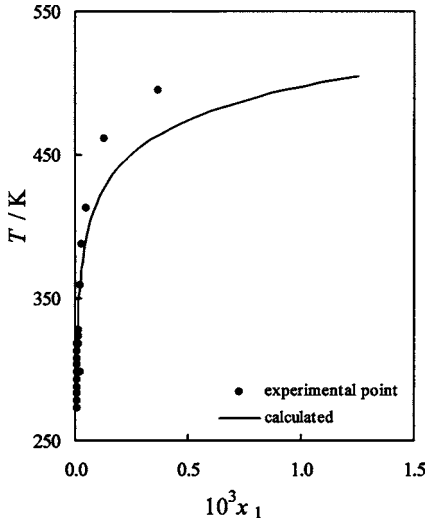

Fig. 3. All the solubility data for propylbenzene (1) in water (2).

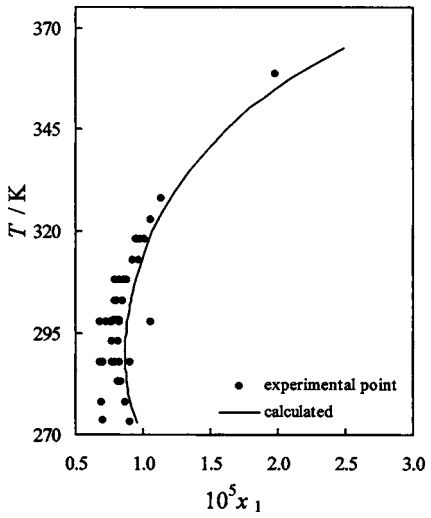

Fig. 4. Recommended and tentative solubility data for propylbenzene (1) in water (2).

Components:	**Original Measurements:**
(1) Propylbenzene; C_9H_{12} ; [103-65-1] (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 Data

The solubility of propylbenzene in water at 25 °C was reported to be $0.0055g(1)/100$ g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is $8.2 \cdot 10^{-6}$.

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; fractionally distilled; b.p. range 157.8 °C–158.1 °C.
(2) Not specified.

Estimated Error:

Not specified.

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001).

Variables:
Temperature: 273.65 K–328.15 K

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

Experimental Data

Solubility of propylbenzene 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	3.87	4.66	6.98
278.15	3.81	4.58	6.86
288.15	3.73	4.49	6.73
298.15	4.01	4.83	7.24
308.25	4.34	5.24	7.86
318.15	5.19	6.31	9.46
328.15	6.19	7.57	11.34

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 98%; purity confirmed by liquid and gas chromatography was >99%; used as received.
(2) Distilled and treated by a Milli-Q water purification system.

Estimated Error:
Temperature: ± 0.01 K.

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Fühner, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).

Variables:
One temperature: 15 °C

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

Experimental Data

The solubility of propylbenzene in water at 15 °C was reported to be $0.006g(1)$/100 g sln.
The corresponding mole fraction, x_1 , calculated by the compilers is $9 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 mL (2) until a completely clear solution was no longer obtained at the experimental temperature.

Source and Purity of Materials:
(1) Source not specified; commercial grade; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Zh. Fiz. Khim. **38**, 805 (1964).

Variables:
Temperature: 85.8 °C–222.0 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of propylbenzene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln
85.8	1.98	0.0132
114.5	2.49	0.0166
140.5	4.81	0.0321
188.0	13.04	0.087
222.0	36.8	0.245

Auxiliary Information

Method/Apparatus/Procedure:
The measurements were made in sealed glass tubes. No details were reported in the paper.

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

Estimated Error:
Not specified.

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(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 Data

The solubility of propylbenzene in water at 25 °C was reported to be 0.12$g(1)$/L sln and 0.001 mol (1)/L sln.

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 from spectra.

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

Estimated Error:
Not specified.

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy **2**, 170 (1975).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of propylbenzene in water at 25 °C was reported to be 0.070 mg (1)/mL sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $0.0070g(1)/100$ g sln and $1.05 \cdot 10^{-5}$. The assumption that 1.00 mL sln = 1.00 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by glc. A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G. column operated at 90 °C–140 °C.

Source and Purity of Materials:
(1) Described in Krasnoshchekova and Gubergrits.[1]
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.

References:
[1]P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(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: 10.0–45.0 °C

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

Experimental Data

Solubility of propylbenzene in water

t/°C	$10^4 \cdot$ mol(1)/L sln	$g(1)/100$ g sln (compilers)	$10^5 \cdot x_1$ (compilers)
10.0	4.47±0.15	0.00537	0.805
15.0	4.35±0.12	0.00523	0.784
20.0	4.52±0.11	0.00544	0.816
25.0	4.43±0.10	0.00534	0.800
30.0	4.37±0.16	0.00527	0.791
35.0	4.71±0.30	0.00569	0.854
40.0	5.32±0.27	0.00644	0.966
45.0	5.54±0.12	0.00672	1.008

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by the technique reported in May *et al.*[1] and DeVoe *et al.*[2] 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.% 3–5 measurements at each temperature were made.

Source and Purity of Materials:
(1) Albany Internationals Chemicals Division; used as received; purity >99% by glc.
(2) HPCL 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) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of propylbenzene in water

t/°C	$10^6 \cdot x_1$ (compiler)[a]	$10^3 \cdot g(1)$/100 g sln[a] (compiler)	$10^4 \cdot$ mol(1)/L sln
15	6.99	4.66	3.88±0.15
25	7.64	5.10	4.23±0.12
35	8.25	5.50	4.55±0.07
45	9.61	6.41	5.28±0.17

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostated flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, S. Arakawa, M. Araki, and T. Deguchi, Bull. Chem. Soc. Jpn. **57**, 1539 (1984).

Variables:
One temperature: 25 °C

Prepared By:
G. T. Hefter

Experimental Data

The solubility of propylbenzene in water at 25 °C was reported to be $3.76 \cdot 10^{-4}$ mol (1)/L sln.

Assuming a solution density of 1.00 kg/L this corresponds to a solubility of $4.52 \cdot 10^{-3}$ $g(1)$/100 g sln, $x_1 = 6.78 \cdot 10^{-6}$, calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus used is described in detail in Sanemasa *et al.*[1] The method involves the introduction of solute vapor (1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analyzed by solvent extraction-UV spectrophotometry

Source and Purity of Materials:
(1) Analytical reagent grade source and purity not stated, used without further purification.
(2) Deionized and redistilled; no further details given.

Estimated Error:
Not specified.

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

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of propylbenzene in water

t/°C	mol (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
25.0	4.15×10^{-4}	5.00×10^{-3}	7.50×10^{-6}

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The apparatus used for preparing aqueous solutions saturated with hydrocarbon vapor was the same as that previously reported in Ref. 1. The method was based on the introduction of gas phase (1) (by bubbling air through the mixture using circulating pump in a closed system) into 100 mL of water. After 10 min (at circulation rate of vapor of 1.5 L/min) equilibrium was attained, and a 30 mL portion of the saturated aqueous solution was transferred into three separatory funnels with 5 mL of toluene. Mixtures were analyzed by gas chromatography.

Source and Purity of Materials:
(1) Source not specified; analytical reagent grade; purity 97%; used as received.
(2) Deionized and redistilled.

Estimated Error:
Temperature: ±0.1 °C.

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

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Kitamura, and Y. Taniguchi, J. Phys. Chem. **93**, 4931 (1989).

Variables:
Temperature: 25.00 °C
Pressure: 0.1–400 MPa

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

Experimental Data

Solubility of propylbenzene in water

t/°C	P/MPa	mol (1)/L sln	x_p/x_0	$10^4\cdot g$(1)/100 g sln (compilers)	$10^5 x_1$ (compilers)
25.00	0.1	$7.7\cdot10^{-4}$	1	0.927	1.39
	25		1.073	0.947	1.42
	50		1.114	1.034	1.55
	100		1.162	1.081	1.62
	150		1.164	1.081	1.62
	200		1.137	1.054	1.58
	250		1.101	1.021	1.53
	300		1.043	0.967	1.45
	350		0.986	0.914	3.33
	400		0.932	0.867	3.13

x_p/x_0 = relation of solubilities at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water and a few drops of propylbenzene were placed in a high pressure optical cell with a Teflon ball for stirring as described in Sawamura *et al.*[1] The sample was pressurized and shaken in a thermoregutated water bath for 5 h. The absorbance was measured with a Hitachi Model 340 double-beam spectrophotometer.

Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1] The solubility was calculated through the Beer-Lambert law. The ratios of the solubility at high and atmospheric pressures are the average of at least 3 measurements.

Source and Purity of Materials:
(1) Nacalai Tesque, Co.; shaken successively with H_2SO_4, Na_2CO_3 aq, H_2O, dried over $MgSO_4$, distilled.
(2) Not specified.

Estimated Error:
Temperature: ±0.01 °C.

References:
[1]S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Sol. Chem. **16**, 649 (1987).

Components:
(1) Propylbenzene; C_9H_{12}; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Nagaoka, and T. Machikawa, J. Phys. Chem. B **105**, 2429 (2001).

Variables:
Temperature: 273.2–323.2 K
Pressure: 0.1–400 MPa

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

Experimental Data

Solubility of propylbenzene in water

T/K	P/MPa	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
273.2	0.1	0.006011	0.901
278.2	0.1	0.005771	0.865
283.2	0.1	0.005591	0.838
288.2	0.1	0.005491	0.823
293.2	0.1	0.005444	0.816
298.2	0.1	0.005491	0.823
303.2	0.1	0.005611	0.841
308.2	0.1	0.005831	0.874
313.2	0.1	0.006124	0.918
318.2	0.1	0.006551	0.982
323.2	0.1	0.007052	1.057
298.2	25	0.005891	0.883
313.2	25	0.006518	0.977
273.2	50	0.006451	0.967
283.2	50	0.006238	0.935
298.2	50	0.006118	0.917
313.2	50	0.006798	1.019
323.2	50	0.007659	1.148
273.2	100	0.006651	0.997
283.2	100	0.006431	0.964
298.2	100	0.006378	0.956
313.2	100	0.007192	1.078
323.2	100	0.008119	1.217
273.2	150	0.006725	1.008
283.2	150	0.006531	0.979
298.2	150	0.006391	0.958
313.2	150	0.007385	1.107
323.2	150	0.008359	1.253
273.2	200	0.006551	0.982
283.2	200	0.006465	0.969
298.2	200	0.006245	0.936
313.2	200	0.007479	1.121
323.2	200	0.008426	1.263
273.2	250	0.006371	0.955
283.2	250	0.006251	0.937
298.2	250	0.006044	0.906
313.2	250	0.007432	1.114
323.2	250	0.008586	1.287
273.2	300	0.006124	0.918
283.2	300	0.005924	0.888
298.2	300	0.005724	0.858
313.2	300	0.007312	1.096
323.2	300	0.008426	1.263
273.2	350	0.005844	0.876
283.2	350	0.005637	0.845
298.2	350	0.005411	0.811
313.2	350	0.007072	1.060
323.2	350	0.008052	1.207
273.2	400	0.005517	0.827
283.2	400	0.005337	0.800
298.2	400	0.005117	0.767
313.2	400	0.006812	1.021
323.2	400	0.007779	1.166

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water and a few drops of benzene were placed in a high pressure optical cell with a Teflon ball for stirring and described in Sawamura *et al.*[1] The sample was pressurized and shaken in a thermoregutated water bath for a few days. The absorbance was measured at the absorption maximum around 260. Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1,2] The solubility was calculated on the basis of measurements and recommended solubility value at 298.15 K and 0.1 MPa reported in Sawamura *et al.*[3]

Source and Purity of Materials:
(1) Nacalai Tesque, Co.; shaken successively with H_2SO_4, Na_2CO_3 aq, H_2O, dried over $MgSO_4$, distilled; Sawamura *et al.*[2]
(2) Deionized; distilled over trace of $KMnO_4$, Sawamura *et al.*[2]

Estimated Error:
Temperature: ±0.1 K (compilers).

References:
[1]S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Sol. Chem. **16**, 649 (1987).
[2]S. Sawamura, K. Kitamura, and Y. Taniguchi, J. Phys. Chem. **93**, 4931 (1989).
[3]D. G. Shaw, ed., *IUPAC Solubility Data Series*, Vol. 37 (Pergamon, New York, 1989).

Components:	**Original Measurements:**
(1) Propylbenzene; C_9H_{12} ; [103-65-1] (2) Water; H_2O; [7732-18-5]	R. S. Stearns, H. Oppenheimer, E. Simon, and W. D. Harkins, J. Chem. Phys. **15**, 496 (1947).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and D. G. Shaw

Experimental Data

The solubility of propylbenzene in water at 25 °C was reported to be $0.012g(1)/100$ g sln.

The corresponding mole fraction, x_1, calculated by the compiler is $1.8 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

Mixtures of (1) in (2) of known composition were shaken for at least 48 h. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±3 °C.

Components:	**Original Measurements:**
(1) Propylbenzene; C_9H_{12} ; [103-65-1] (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 Data

Solubility of propylbenzene in water

t/°C	mol (1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
25.0	$4.34 \cdot 10^{-4}$	$5.23 \cdot 10^{-3}$	$7.84 \cdot 10^{-6}$

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 water into the inlet of the coated column and 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).

Components:
(1) Propylbenzene; C_9H_{12} ; [103-65-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (U.S.) **86**, 361 (1981).

Variables:
Temperature: 15.0 °C–30.0 °C

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

Experimental Data

Solubility of propylbenzene 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)
15.0[a]	4.26±0.05	5.12	7.68
20.0[a]	4.25±0.12	5.12	7.67
23.0[b]	4.27±0.06	5.14	7.71
25.0[a]	4.32±0.02	5.20	7.80
30.0[a]	4.45±0.05	5.37	8.05

Auxiliary Information

Method/Apparatus/Procedure:
The generator column technique (a) and stir-flask equibration method (b) were used. In (a), the dynamic coupled column liquid chromatography method, described in May *et al.*,[1,2] generated saturated solutions by pumping water through a column packed with glass beads that had been coated with propylbenzene. The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatography process. In (b) a mixture of 100 mL of water and 4 mL of propylbenzene after 16 h of stirring and equilibration was analyzed by the HPLC method. Each reported solubility is a mean value of 2–4 measurements.

Source and Purity of Materials:
(1) Chemical Samples Co.; purity 99.9%.
(2) Distilled water.

Estimated Error:
Temperature: ±1 °C.
Solubility: as above (mean deviation).

References:
[1]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

2.6. 1,2,3-Trimethylbenzene (hemimellitene)+Water*

Components:
(1) 1,2,3-Trimethylbenzene (hemimellitene); C_9H_{12} ; [526-73-8]
(2) Water; H_2O; [7732-18-5]

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

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

The experimental solubility data for (1) in (2) have been investigated by Sanemasa *et al.*[1] at 288–318 K, Sutton and Calder,[3] and Tewari *et al.*[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:

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

where $\ln x_{\min,1} = -11.33$, $D = 44.96$, and $T_{\min} = 290$.

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 categories.

All the experimental and reference data are listed in Table 6 and shown in Fig. 5. The data of Sanemasa *et al.*,[1] Sutton and Calder,[2]

TABLE 6. Experimental values for solubility of 1,2,3-trimethylbenzene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative)	Reference values $x_1 \pm 30\%$
288.2	$8.97 \cdot 10^{-6}$ (T; Ref. 1)	$1.2 \cdot 10^{-5}$
298.2	$9.40 \cdot 10^{-6}$ (R; Ref. 1), $1.13 \cdot 10^{-5}$ (R; Ref. 2)	$1.2 \cdot 10^{-5}$
	$9.85 \cdot 10^{-6}$ (R; Ref. 3)	
308.2	$1.08 \cdot 10^{-5}$ (T; Ref. 1)	$1.3 \cdot 10^{-5}$
318.2	$1.28 \cdot 10^{-5}$ (T; Ref. 1)	$1.4 \cdot 10^{-5}$

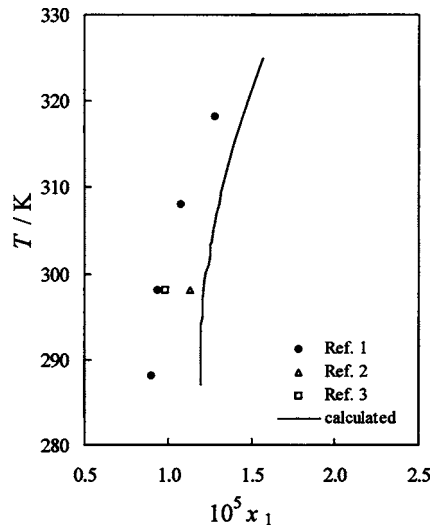

Fig. 5. All the solubility data for 1,2,3-trimethylbenzene (1) in water (2).

and Tewari *et al.*[3] at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. All the remaining data are in good agreement agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:

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

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

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

Components:	**Original Measurements:**
(1) 1,2,3-Trimethylbenzene; C_9H_{12} ; [526-73-8] (2) Water; H_2O; [7732-18-5]	I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
Variables:	**Prepared By:**
Temperature: 15 °C–45 °C	G. T. Hefter

Experimental Data

Solubility of 1,2,3-trimethylbenzene in water

t/°C	$10^6 \cdot x_1$ (compiler)[a]	$10^3 \cdot g(1)$/100 g sln[a] (compiler)	$10^4 \cdot$ mol(1)/L sln
15	8.97	5.99	4.98±0.19
25	9.40	6.27	5.20±0.32
35	10.8	7.22	5.97±0.41
45	12.8	8.52	7.02±0.19

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostated flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:

Temperature: ±0.01 °C.
Solubility: see table, type of error not specified.

References:

[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).

[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) 1,2,3-Trimethylbenzene; C_9H_{12} ; [526-73-8]
(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 Data

The solubility of 1,2,3-trimethylbenzene in water at 25 °C was reported to be 75.2 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are $0.00752g(1)/100$ g sln and $1.126 \cdot 10^{-5}$.

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 purified by distillation; 94.4% purity determined by gas chromatography.
(2) Distilled.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 0.6 (std. dev. of the mean for six replicates).

Components:
(1) 1,2,3-Trimethylbenzene; C_9H_{12} ; [526-73-8]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of 1,2,3-trimethylbenzene in water

t/°C	mol (1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
25.0	$5.45 \cdot 10^{-4}$	$6.57 \cdot 10^{-3}$	$9.85 \cdot 10^{-6}$

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 water into the inlet of the coated column and was then analyzed by hplc. 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 >90 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).

2.7. 1,2,4-Trimethylbenzene (pseudocumene)+Water*

Components:
(1) 1,2,4-Trimethylbenzene (pseudocumene); C_9H_{12} ; [95-63-6]
(2) Water; H_2O; [7732-18-5]

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

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

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

Author (s)	T/K	Author (s)	T/K
McAuliffe[1]	298	Sanemasa *et al.*[3]	288–318
Price[2]	298	Sutton and Calder[4]	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:

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

where $\ln x_{\min,1} = -11.72$, $D = 46.58$, and $T_{\min} = 290$.

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 categories.

All the experimental and reference data are listed in Table 7 and shown in Fig. 6. The data of McAuliffe,[1] Price,[2] Sanemasa *et al.*,[3] and Sutton and Calder[4] at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. All the remaining data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

TABLE 7. Experimental values for solubility of 1,2,4-trimethylbenzene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative)	Reference values $x_1 \pm 30\%$
288.2	$7.84 \cdot 10^{-6}$ (T; Ref. 3)	$8.2 \cdot 10^{-6}$
298.2	$8.50 \cdot 10^{-6}$ (R; Ref. 1), $7.77 \cdot 10^{-6}$ (R; Ref. 2), $8.48 \cdot 10^{-6}$ (R; Ref. 3), $8.83 \cdot 10^{-6}$ (R; Ref. 4)	$8.3 \cdot 10^{-6}$
308.2	$9.32 \cdot 10^{-6}$ (T; Ref. 3)	$8.9 \cdot 10^{-6}$
318.2	$1.04 \cdot 10^{-5}$ (T; Ref. 3)	$9.9 \cdot 10^{-6}$

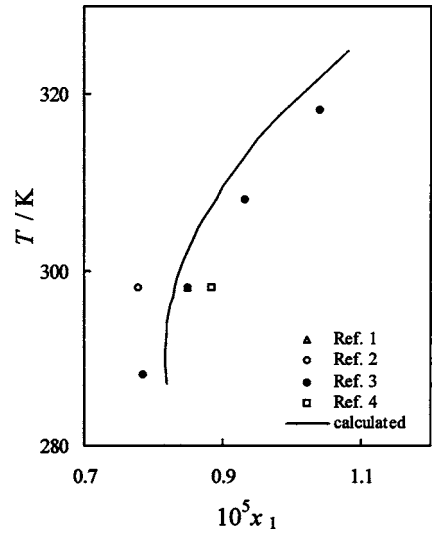

Fig. 6. All the solubility data for 1,2,4-trimethylbenzene (1) in water (2).

Rejected Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[5] are independent data. Therefore these data are Rejected.

References:

[1]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[2]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[3]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[4]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[5]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Components:	Original Measurements:
(1) 1,2,4-Trimethylbenzene; C_9H_{12} ; [95-63-6] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of 1,2,4-trimethylbenzene in water at 25 °C was reported to be 57 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are $0.0057g(1)/100$ g sln and $8.5\cdot10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjuction with a flame-ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 4 mg (1)/kg (2) (std. dev. of mean).

Components:	Original Measurements:
(1) 1,2,4-Trimethylbenzene; C_9H_{12} ; [95-63-6] (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 Data

The solubility of 1,2,4-trimethylbenzene in water at 25 °C and at system pressure was reported to be 51.9 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $0.00519g(1)/100$ g sln and $7.77\cdot10^{-6}$.

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: ±1.2 mg(1)/kg(2).

Components:
(1) 1,2,4-Trimethylbenzene; C_9H_{12} ; [95-63-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of 1,2,4-trimethylbenzene in water

t/°C	$10^6 \cdot x_1$ (compiler)[a]	$10^3 \cdot g(1)$/100 g sln (compiler)[a]	$10^4 \cdot$ mol(1)/L sln
15	7.84	5.23	4.35±0.12
25	8.48	5.65	4.69±0.07
35	9.32	6.21	5.14±0.20
45	10.4	6.93	5.71±0.07

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 95.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) 1,2,4-Trimethylbenzene; C_9H_{12} ; [95-63-6]
(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 Data

The solubility of 1,2,4-trimethylbenzene in water at 25 °C was reported to be 59.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00590 $g(1)$/100 g sln and $8.83 \cdot 10^{-6}$.

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: 0.8 mg (1)/kg (2) (std. dev. of the mean for six replicates).

2.8. 1,3,5-Trimethylbenzene (mesitylene)+Water*

Components:
(1) 1,3,5-Trimethylbenzene (mesitylene); C_9H_{12} ; [108-67-8]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of 1,3,5-Trimethylbenzene (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	Sanemasa *et al.*[6]	288–318
Booth and Everson[2]	298	Sanemasa *et al.*[7]	288–318
Chen and Wagner[3]	303–373 (136–238 kPa)	Sutton and Calder[8]	298
Guseva and Parnov[5]	391–484	Vesala[9]	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:

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

where $\ln x_{\min,1} = -11.85$, $D = 47.15$, and $T_{\min} = 290$.

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 listed in Table 8.

All the experimental and reference data are listed in Table 9 and shown in Fig. 7. The Recommended and Tentative data are shown in Fig. 8.

TABLE 8. The data categories for solubility of 1,3,5-trimethylbenzene (1) in water (2)

T/K	Recommended (data in good agreement with each other and with the reference data)	Tentative (data in good agreement with the reference data)	Doubtful (data in poor agreement with the reference data)
288.2		Sanemasa *et al.*[6] Sanemasa *et al.*[7]	
298.0		Vesala[9]	
298.2	Sanemasa *et al.*[6] Sanemasa *et al.*[7] Sutton and Calder[8]		Andrews and Keefer[1] Booth and Everson[2]
303.2		Chen and Wagner[3]	
308.2		Sanemasa *et al.*[6] Sanemasa *et al.*[7]	
313.2		Chen and Wagner[3]	
318.2		Sanemasa *et al.*[6] Sanemasa *et al.*[7]	
323.2		Chen and Wagner[3]	
333.2		Chen and Wagner[3]	
343.2		Chen and Wagner[3]	
353.2			Chen and Wagner[3]
363.2		Chen and Wagner[3]	
373.2		Chen and Wagner[3]	
391.2			Guseva and Parnov[5]
417.2			Guseva and Parnov[5]
460.2			Guseva and Parnov[5]
484.2			Guseva and Parnov[5]

TABLE 9. Experimental values for solubility of 1,3,5-trimethylbenzene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
288.2		$6.82\cdot10^{-6}$ (T; Ref. 6), $6.90\cdot10^{-6}$ (T; Ref. 7)	$7.2\cdot10^{-6}$
298.0		$5.91\cdot10^{-6}$ (T; Ref. 9)	$7.3\cdot10^{-6}$
298.2		$1.45\cdot10^{-5}$ (D; Ref. 1), $3.00\cdot10^{-5}$ (D; Ref. 2), $7.41\cdot10^{-6}$ (R; Ref. 6), $7.50\cdot10^{-6}$ (R; Ref. 7), $7.22\cdot10^{-6}$ (R; Ref. 8)	$7.3\cdot10^{-6}$
303.2	136 (Ref. 3)	$9.58\cdot10^{-6}$ (T; Ref. 3)	$7.5\cdot10^{-6}$
308.2		$8.11\cdot10^{-6}$ (T; Ref. 6), $8.22\cdot10^{-6}$ (T; Ref. 7)	$7.8\cdot10^{-6}$
313.2	136 (Ref. 3)	$1.00\cdot10^{-5}$ (T; Ref. 3)	$8.2\cdot10^{-6}$
318.2		$8.46\cdot10^{-6}$ (T; Ref. 6), $8.83\cdot10^{-6}$ (T; Ref. 7)	$8.7\cdot10^{-6}$
323.2	136 (Ref. 3)	$1.11\cdot10^{-5}$ (T; Ref. 3)	$9.3\cdot10^{-6}$
333.2	136 (Ref. 3)	$1.36\cdot10^{-5}$ (T; Ref. 3)	$1.1\cdot10^{-5}$
343.2	136 (Ref. 3)	$1.66\cdot10^{-5}$ (T; Ref. 3)	$1.3\cdot10^{-5}$
353.2	136 (Ref. 3)	$2.09\cdot10^{-5}$ (D; Ref. 3)	$1.6\cdot10^{-5}$
363.2	204 (Ref. 3)	$2.45\cdot10^{-5}$ (T; Ref. 3)	$2.0\cdot10^{-5}$
373.2	238 (Ref. 3)	$2.91\cdot10^{-5}$ (T; Ref. 3)	$2.5\cdot10^{-5}$
391.2		$1.00\cdot10^{-5}$ (D; Ref. 5)	$4.05\cdot10^{-5}$
417.2		$1.90\cdot10^{-5}$ (D; Ref. 5)	$8.33\cdot10^{-5}$
460.2		$6.10\cdot10^{-5}$ (D; Ref. 5)	$2.94\cdot10^{-4}$
484.2		$1.17\cdot10^{-4}$ (D; Ref. 5)	$6.02\cdot10^{-4}$

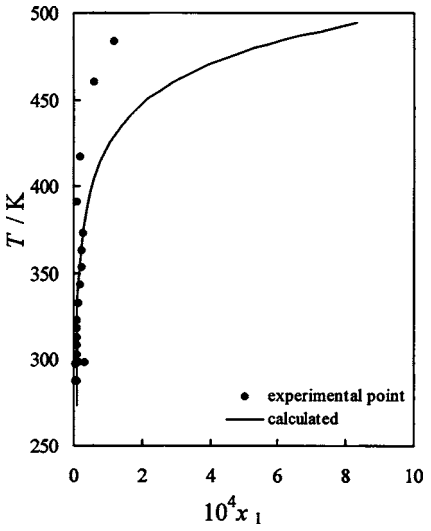

Fig. 7. All the solubility data for 1,3,5-trimethylbenzene (1) in water (2).

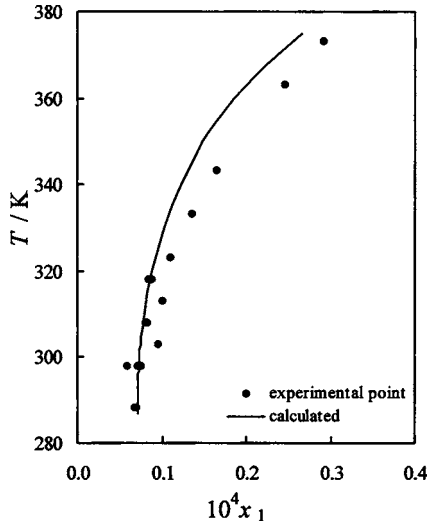

Fig. 8. Recommended and tentative solubility data for 1,3,5-trimethylbenzene (1) in water (2).

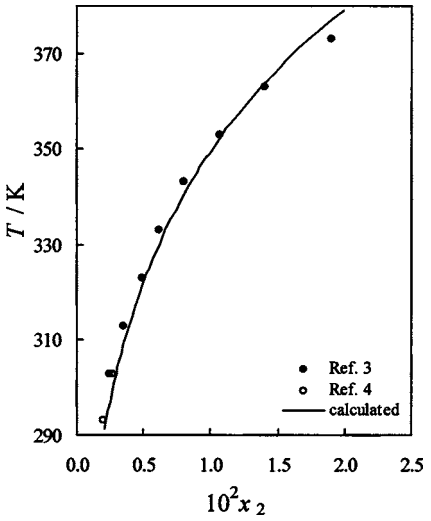

Fig. 9. All the solubility data for water (2) in 1,3,5-trimethylbenzene (1).

Critical Evaluation of the Solubility of Water (2) in 1,3,5-Trimethylbenzene (1)

The experimental solubility data for (2) in (1) have been investigated Chen and Wagner[3] at 303 K–373 K and 136 kPa–238 kPa, and Englin *et al.*[4] at 293K–313 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:

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

where $d_1 = -0.307$, $d_2 = -2.743$, $d_3 = 0.101$, $d_4 = -6.560$, and $T_r = T/577.1$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1,3,5-trimethylbenzene 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 categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 10 and shown in Fig. 9. The data of Chen and Wagner,[3] and Englin *et al.*[4] at 303 and 313 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. All the remaining data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

TABLE 10. Experimental values for solubility of water (2) in 1,3,5-trimethylbenzene (1)

T/K	P/kPa	Experimental values x_2 (R=recommended, T=tentative)	Reference values $x_2 \pm 30\%$
293.2		$1.94 \cdot 10^{-3}$ (T; Ref. 4)	$2.2 \cdot 10^{-3}$
303.2	136 (Ref. 3)	$2.47 \cdot 10^{-3}$ (R; Ref. 3), $2.62 \cdot 10^{-3}$ (R; Ref. 4)	$3.0 \cdot 10^{-3}$
313.2	136 (Ref. 3)	$3.50 \cdot 10^{-3}$ (R; Ref. 3), $3.45 \cdot 10^{-3}$ (R; Ref. 4)	$3.9 \cdot 10^{-3}$
323.2	136 (Ref. 3)	$4.88 \cdot 10^{-3}$ (T; Ref. 3)	$5.1 \cdot 10^{-3}$
333.2	136 (Ref. 3)	$6.09 \cdot 10^{-3}$ (T; Ref. 3)	$6.7 \cdot 10^{-3}$
343.2	136 (Ref. 3)	$7.97 \cdot 10^{-3}$ (T; Ref. 3)	$8.5 \cdot 10^{-3}$
353.2	136 (Ref. 3)	$1.06 \cdot 10^{-2}$ (T; Ref. 3)	$1.1 \cdot 10^{-2}$
363.2	204 (Ref. 3)	$1.40 \cdot 10^{-2}$ (T; Ref. 3)	$1.4 \cdot 10^{-2}$
373.2	238 (Ref. 3)	$1.90 \cdot 10^{-2}$ (T; Ref. 3)	$1.7 \cdot 10^{-2}$

Rejected and Inaccessible Data

The data reported by Alwani and Schneider[10] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
[2]H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
[3]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).
[4]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[5]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).
[6]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).
[7]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[8]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[9]A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).
[10]Z. Alwani and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **73**, 294 (1969).

Components:	Original Measurements:
(1) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8] (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 Data

The solubility of 1,3,5-trimethylbenzene in water at 25 °C was reported to be 0.0097 $g(1)$/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $1.45 \cdot 10^{-5}$.

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. white label; fractionally distilled; b.p. 165.0 °C.
(2) Not specified.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8] (2) Water; H_2O; [7732-18-5]	H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of 1,3,5-trimethylbenzene in water at 25 °C was reported to be less than 0.02 $g(1)$/100 mL(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are <0.02 $g(1)$/100 g sln and $<3.0 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

Stoppered Babcock tubes with neck 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, the 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) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).

Variables:
Temperature: 303.15 K–373.15 K
Pressure: 1.36 bar–2.38 bar

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

Experimental Data

Solubility of 1,3,5-trimethylbenzene in water

T/K	P/bar	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
303.15	1.36	0.00639	0.958 ± 0.053
313.15	1.36	0.00667	1.00 ± 0.05
323.15	1.36	0.00740	1.11 ± 0.06
333.15	1.36	0.00907	1.36 ± 0.07
343.15	1.36	0.01107	1.66 ± 0.12
353.15	1.36	0.01394	2.09 ± 0.06
363.15	2.04	0.01634	2.45 ± 0.06
373.15	2.38	0.01941	2.91 ± 0.06

Solubility of water in 1,3,5-trimethylbenzene

T/K	P/bar	$g(2)$/100 g sln (compilers)	$10^2 \cdot x_2$
303.15	1.36	0.0371	0.247 ± 0.009
313.15	1.36	0.0526	0.350 ± 0.019
323.15	1.36	0.0734	0.488 ± 0.018
333.15	1.36	0.0918	0.609 ± 0.017
343.15	1.36	0.1203	0.797 ± 0.028
353.15	1.36	0.1603	1.06 ± 0.03
363.15	2.04	0.2124	1.40 ± 0.07
373.15	2.38	0.2895	1.90 ± 0.04

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A continuous flow equilibrium apparatus for mutual solubility measurements, Chen and Wagner,[1] was used. Samples were collected in 25 mL vials and 60 and 120 mL bottles containing anhydrous ethanol or methylene chloride as a 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 4–7 replicate determinations.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; purity >98.5 mole %; used as received.
(2) Distilled and deionized 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:
(1) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8]
(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 °C–40 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in 1,3,5-trimethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
20	1.94	0.0291
30	2.62	0.0393
40	3.45	0.0519

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) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).

Variables:
Temperature: 118 °C–211 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of 1,3,5-trimethylbenzene in water

t/°C	$10^4 \cdot x_1$	$g(1)$/100 g sln
118	0.10	0.007
144	0.19	0.013
187	0.61	0.041
211	1.17	0.078

Auxiliary Information

Method/Apparatus/Procedure:
The measurements were made in sealed glass tubes. No details were reported in the paper.

Source and Purity of Materials:
(1) Source not specified; $n_D^{20} = 1.49945$.
(2) Doubly distilled.

Estimated Error:
Not specified.

Components:
(1) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of 1,3,5-trimethylbenzene in water

T/K	$10^6 \cdot x_1$ [a]	$g(1)$/100 g sln[a]	$g(1)$/L
15	6.82	0.00456	0.0456 ± 0.0010
25	7.41	0.00495	0.0495 ± 0.0015
35	8.11	0.00542	0.0542 ± 0.0033
45	8.46	0.00565	0.0565 ± 0.0031

[a]Calculated by compiler assuming a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted separatory funnel, respectively. The solute vapor, generated by bubbling air through the liquid solute, was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous solution were transferred into funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported. The solubility runs were made such that the temperature of solute reservoir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.

Source and Purity of Materials:
(1) Analytical reagent grade used as purchased.
(2) Redistilled.

Estimated Error:
Solubility: given above.

Components:
(1) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of 1,3,5-trimethylbenzene in water

t/°C	$10^6 \cdot x_1$ (compiler)[a]	$10^3 \cdot g(1)$/100 g sln (compiler)[a]	$10^4 \cdot$mol(1)/L sln
15	6.90	4.60	3.83±0.15
25	7.50	5.00	4.15±0.22
35	8.22	5.49	4.55±0.23
45	8.83	5.89	4.85±0.32

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8]
(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 Data

The solubility of 1,3,5-trimethylbenzene in water at 25 °C was reported to be 48.2 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00482 $g(1)$/100 g sln and $7.22 \cdot 10^{-6}$.

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 (std. dev. of the mean for six replicates).

2.9. 1-Nonyne+Water

Components:
(1) 1-Nonyne; C_9H_{16} ; [3452-09-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

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

Experimental Data

The solubility of 1-nonyne in water at 25 °C was reported to be 7.2 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00072 $g(1)$/100 g sln and $1.0 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjuction with a flame ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ± 1.5 °C.
Solubility: 0.5 mg (1)/kg (2) (std. dev. of mean).

Components:
(1) 1,3,5-Trimethylbenzene; C_9H_{12} ; [108-67-8]
(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 Data

Solubility of 1,3,5-trimethylbenzene in water

T/K	mol (1)/g (2)	$g(1)$/100 g sln (compilers)	x_1 (compilers)
298.15	$(3.28 \pm 0.05) \cdot 10^{-7}$	$3.94 \cdot 10^{-5}$	$5.91 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The equilibration was carried out in a modified vessel (Franks *et al.*)[1] equipped with a magnetic stirrer. The temperature of the water bath was maintained within ± 0.05 K. Equilibrium was obtained after 48 h and then samples were analyzed by spectrophotometry. At least 5 parallel determinations were performed

Source and Purity of Materials:
(1) Commercial analytical grade reagent; purity >99% by glc; distilled through a column.
(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).

2.10. Butylcyclopentane+Water

Components:
(1) Butylcyclopentane; C_9H_{18} ; [2040-95-1]
(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 °C–30 °C

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

Experimental Data

Solubility of water in butylcyclopentane

t/°C	$10^{-4} \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.93	0.0056
20	6.66	0.0095
30	10.58	0.0151

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.

2.11. 1-Nonene+Water

Components:
(1) 1-Nonene; C_9H_{18} ; [124-11-8]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of 1-nonene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$8.85 \cdot 10^{-6}$	$1.121 \cdot 10^{-4}$	$1.600 \cdot 10^{-7}$

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 water into the inlet of the coated column and was then analyzed by 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).

2.12. 1,1,3-Trimethylcyclohexane+Water

Components:
(1) 1,1,3-Trimethylcyclohexane; C_9H_{18} ; [3073-66-3]
(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 Data

The solubility of 1,1,3-trimethylcyclohexane in water at 25 °C and at system pressure was reported to be 1.77 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $1.77 \cdot 10^{-4}$ $g(1)$/100 g sln and $2.53 \cdot 10^{-7}$.

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: ±0.05 mg(1)/kg(2).

2.13. 2,6-Dimethylheptane+Water

Components:
(1) 2,6-Dimethylheptane; C_9H_{20} ; [1072-05-5]
(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 °C–50 °C

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

Experimental Data

Solubility of water in 2,6-dimethylheptane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.77	0.0053
20	6.48	0.0091
30	11.39	0.0160
40	21.40	0.0301
50	33.02	0.0465

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.

2.14. 2-Methyloctane+Water

Components:	**Original Measurements:**
(1) 2-Methyloctane; C_9H_{20} ; [3221-61-2] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 10 °C–30 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Data

Solubility of water in 2-methyloctane

t/°C	$10^{-4} \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.70	0.0052
20	6.41	0.0090
30	11.10	0.0156

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
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	(1) Not specified. (2) Not specified. **Estimated Error:** Not specified.

2.15. 3-Methyloctane+Water

Components:	**Original Measurements:**
(1) 3-Methyloctane; C_9H_{20} ; [2216-33-3] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 10 °C–30 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Data

Solubility of water in 3-methyloctane

t/°C	$10^{-4} \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.56	0.0050
20	6.20	0.0087
30	11.03	0.0155

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
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	(1) Not specified. (2) Not specified. **Estimated Error:** Not specified.

2.16. 4-Methyloctane+Water

Components:
(1) 4-Methyloctane; C_9H_{20} ; [2216-34-4]
(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 Data

The solubility of 4-methyloctane 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 are $1.15 \cdot 10^{-5}$ $g(1)/100$ g sln and $1.6 \cdot 10^{-8}$.

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).

2.17. Nonane+Water*

Components:
(1) Nonane; C_9H_{20} ; [111-84-2]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Nonane (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
Jonsson *et al.*[2]	288 and 293	McAuliffe[4]	298
Krasnoshchekova[3]	298	Price[5]	298–410

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:

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

where $\ln x_{\min,1} = -17.95$, $\Delta_{sln}C_p/R = 70.7$, and $T_{min} = 306$ 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 categories.

All the experimental and reference data are listed in Table 11 and shown in Fig. 10. The data of Price[5] at 298 and 372 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 Nanane (1)

The experimental solubility for (2) in (1) have been investigated by Benkovski *et al.*[1] at 303 K, and Schatzberg[6] at 298 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:

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

where $d_1 = -0.240$, $d_2 = -5.636$, $d_3 = -1.029$, $d_4 = -3.056$, and $T_r = T/558.8$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of nonane 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 categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 12. The data of Schatzberg[6] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Benkovski *et al.*[1] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

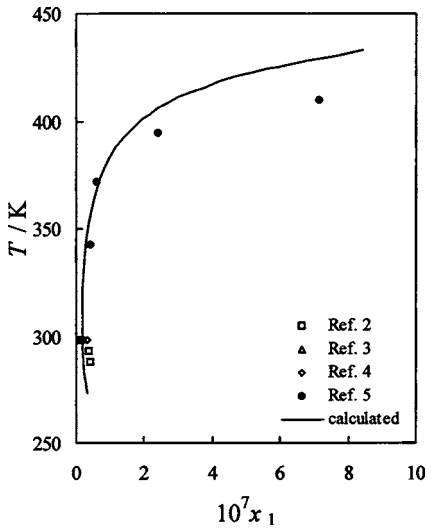

Fig. 10. All the solubility data for nonane (1) in water (2).

TABLE 11. Experimental values for solubility of nonane (1) in water (2)

T/K	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
288.2	$4.05 \cdot 10^{-8}$ (D; Ref. 2)	$2.1 \cdot 10^{-8}$
293.2	$3.81 \cdot 10^{-8}$ (D; Ref. 2)	$2.0 \cdot 10^{-8}$
298.2	$1.00 \cdot 10^{-8}$ (D; Ref. 3), $3.09 \cdot 10^{-8}$ (D; Ref. 4), $1.71 \cdot 10^{-8}$ (T; Ref. 5)	$1.9 \cdot 10^{-8}$
342.9	$4.34 \cdot 10^{-8}$ (D; Ref. 5)	$2.9 \cdot 10^{-8}$
372.3	$5.90 \cdot 10^{-8}$ (D; Ref. 5)	$6.7 \cdot 10^{-8}$
394.5	$2.39 \cdot 10^{-7}$ (D; Ref. 5)	$1.5 \cdot 10^{-7}$
409.8	$7.12 \cdot 10^{-7}$ (D; Ref. 5)	$2.9 \cdot 10^{-7}$

TABLE 12. Experimental values for solubility of water (2) in nonane (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
298.2	$5.6 \cdot 10^{-4}$ (T; Ref. 6)	$6.2 \cdot 10^{-4}$
303.0	$3.2 \cdot 10^{-4}$ (D; Ref. 1)	$7.5 \cdot 10^{-4}$

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[7] are independent data. The data reported by Roof[8] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1]V. G. Benkovski, M. H. Nauruzov, and T. M. Bogoslovskaya, Tr. Inst. Khim. Nefti Prir. Solei, Akad. Nauk Kaz. SSR **2**, 25 (1970).
[2]J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. **9**, 279 (1982).
[3]R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).
[4]C. McAuliffe, Science **163**, 478 (1969).
[5]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[6]P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).
[7]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).
[8]J. G. Roof, J. Chem. Eng. Data **15**, 301 (1970).

Components:	**Original Measurements:**
(1) Nonane; C_9H_{20}; [111-84-2]	J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. **9**, 279 (1982).
(2) Water; H_2O; [7732-18-5]	
Variables:	**Prepared By:**
Temperature: 15 °C–20 °C	G. T. Hefter

Experimental Data

Solubility of nonane in water

t/°C	$10^8 \cdot x_1$ (compiler)	$10^5 \cdot g(1)$/100 g sln (compiler)	mg (1)/kg sln
15	4.05	2.89	0.289
20	3.81	2.72	0.272

Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinite dilution were valid at the saturation pressure of (1).

Auxiliary Information

Method/Apparatus/Procedure:

Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapor concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and entrapped (1) analyzed by gas chromatography. The method and apparatus are described in detail in Vejrosta *et al.*[1]

Source and Purity of Materials:

(1) Fluka, >99%, used as received.
(2) Not specified.

Estimated Error:

Not specified.

References:

[1]J. Vejrosta, J. Novak, and J. A. Jonsson, Fluid Phase Equil. **8**, 25, (1982).

Components:	**Original Measurements:**
(1) Nonane; C_9H_{20}; [111-84-2]	V. G. Benkovski, M. H. Nauruzov, and T. M. Bogoslovskaya, Tr. Inst. Khim. Nefti Prir. Solei, Akad. Nauk Kaz. SSR **2**, 25 (1970).
(2) Water; H_2O; [7732-18-5]	
Variables:	**Prepared By:**
One temperature: 303 K	A. Maczynski

Experimental Data

The solubility of water in nonane at 303 K was reported to be 0.0045 $g(2)$/100 g sln.

The corresponding mole fraction, x_2, value calculated by compiler is 0.00032.

Auxiliary Information

Method/Apparatus/Procedure:

Equal volumes of (1) and (2) were placed in a glass cylinder and periodically shaken for 6 h, then sampled and analyzed by the Karl Fischer method

Source and Purity of Materials:

(1) Source not specified; purified; purity not specified.
(2) Distilled.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Nonane; C_9H_{20} ; [111-84-2] (2) Water; H_2O; [7732-18-5]	R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Data

The solubility of nonane in water at 25 °C was reported to be $x_1 = 1.00 \cdot 10^{-8}$.

The corresponding mass percent calculated by the compiler is $7.1 \cdot 10^{-6}$ $g(1)$/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously 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.	(1) Source not specified; CP reagent; purity not specified. (2) Distilled. **Estimated Error:** Not specified.

Components:	Original Measurements:
(1) Nonane; C_9H_{20} ; [111-84-2] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, Science **163**, 478 (1969).
Variables:	**Prepared By:**
One temperature: 25 °C	F. Kapuku

Experimental Data

The solubility of nonane in water at 25 °C was reported to be 0.220 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $2.2 \cdot 10^{-5}$ $g(1)$/100 g sln and $3.09 \cdot 10^{-8}$.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
(1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of the 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	(1) Not specified. (2) Distilled. **Estimated Error:** Solubility: ± 0.021 mg(1)/kg(2).

Components:
(1) Nonane; C_9H_{20} ; [111-84-2]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 25 °C–136.6 °C

Prepared By:
F. Kapuku

Experimental Data

Solubility of nonane in water at system pressure

t/°C	$10^8 \cdot x_1$ (compiler)	$g(1)$/100 g sln (compiler)	mg (1)/kg (2)
25.0	1.71	0.0000122	0.122±0.007
69.7	4.34	0.0000309	0.309±0.019
99.1	5.90	0.0000420	0.420±0.034
121.3	23.9	0.000170	1.70±0.11
136.6	71.2	0.000507	5.07±025

Auxiliary Information

Method/Apparatus/Procedure:
Room temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured saturation (in 2–4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of a gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified microlinear valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample was then transferred to the gas chromatograph equipped with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Company; 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.
Solubility: range of values given above.

Components:
(1) Nonane; C_9H_{20} ; [111-84-2]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of water in nonane at 25 °C was reported to be 79 mg (2)/kg sln corresponding to a mole fraction, x_2, of $5.6 \cdot 10^{-4}$.

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 of methanol to a dead stop end point using a Beckman KF3 automatic titrimeter.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; research grade; 99.69 mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220–340 nm spectral range.
(2) Distilled and deionized.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: 0–6% (dev. from the mean).

2.18. 2,2,5-Trimethylhexane+Water*

Components:	Evaluators:
(1) 2,2,5-Trimethylhexane; C_9H_{20} ; [3522-94-9]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska,
(2) Water; H_2O; [7732-18-5]	Thermodynamics Data Center, Warsaw, Poland, February, 2004.

Critical Evaluation of the Solubility of 2,2,5-Trimethylhexane (1) in Water (2)

The experimental solubility for (1) in (2) have been investigated by McAuliffe[1] at 298 K and Polak and Lu[2] at 273 K and 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:

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

where: $\ln x_{\min,1} = -16.85$; $\Delta_{sln}C_p/R = 65.0$; $T_{min} = 306$ 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 categories.

All the experimental and reference data are listed in Table 13. The data of Polak and Lu[2] at 273 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of McAuliffe,[1] and Polak and Lu[1] at 298 K are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

TABLE 13. Experimental values for solubility of 2,2,5-trimethylhexane (1) in water (2)

T/K	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$1.11 \cdot 10^{-7}$ (T; Ref. 2)	$8.6 \cdot 10^{-8}$
298.2	$1.62 \cdot 10^{-7}$ (D; Ref. 1), $7.58 \cdot 10^{-8}$ (D; Ref. 2)	$5.7 \cdot 10^{-8}$

Critical Evaluation of the Solubility of Water (2) in 2,2,5-Trimethylhexane (1)

The experimental solubility for (2) in (1) have been investigated by Polak and Lu[1] at 273 and 298 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:

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

where $d_1 = -0.486$, $d_2 = -5.745$, $d_3 = -0.518$, $d_4 = -3.776$, and $T_r = T/543.4$

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 2,2,5-trimethylhexane 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 14. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

TABLE 14. Experimental values for solubility of water (2) in 2,2,5-trimethylhexane (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
273.2	$1.78 \cdot 10^{-4}$ (T; Ref. 2)	$2.1 \cdot 10^{-4}$
298.2	$5.34 \cdot 10^{-4}$ (T; Ref. 2)	$6.7 \cdot 10^{-4}$

References:

[1]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

[2]J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Components:
(1) 2,2,5-Trimethylhexane; C_9H_{20} ; [3522-94-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of 2,2,5-trimethylhexane in water

t/°C	x_1 (compiler)	mg (1)/kg sln
0[a]	$1.11 \cdot 10^{-7}$	0.79[c]
25[b]	$7.58 \cdot 10^{-8}$	0.54[c]

Solubility of water in 2,2,5-trimethylhexane

t/°C	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0[a]	1.78	25[d]
25[b]	5.34	75[e]

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.
The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±4%, (d) ±4.7%, (e) ±3.1% (mean).

Components:
(1) 2,2,5-Trimethylhexane; C_9H_{20} ; [3522-94-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of 2,2,5-trimethylhexane in water at 25 °C was reported to be 1.15 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is $1.62 \cdot 10^{-7}$. The same value is also reported in McAuliffe.[1]

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 mL sample of the (1) saturated water was withdrawn with a Hamilton syringe and injected into the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; 99+% purity; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 0.008 mg (1)/kg sln (std. dev. from mean).

References:
[1]C. McAuliffe, Am. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

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

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