IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater-Revised and Updated. Part 5. C_7 Hydrocarbons with Water and Heavy Water

Volume Editors
Andrzej Maczynski[a)]
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

David G. Shaw[b)]
University of Alaska, Fairbanks, Alaska, USA

Evaluators
Marian Goral and Barbara Wisniewska-Goclowska
Institute of Coal Chemistry, Polish Academy of Sciences, Gliwice, Poland

Compilers
Adam Skrzecz*
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Iwona Owczarek and Krystyna Blazej
Institute of Coal Chemistry, Polish Academy of Sciences, Gliwice, Poland

Marie-Claire Haulait-Pirson
University of Leuven, Leuven, Belgium

Glenn T. Hefter
Murdoch University, Perth, Australia

F. Kapuku
University of Leuven, Leuven, Belgium

Zofia Maczynska
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Andrzej Szafranski
Institute of Industrial Chemistry, Warsaw, Poland

Colin L. Young
University of Melbourne, Parkville, Australia

(Received 11 April 2004; revised manuscript received 10 May 2004; accepted 20 May 2004; published online 16 August 2005)

[a)] Electronic mail: macz@ichf.edu.pl
[b)] Electronic mail: DavidShaw@post.harvard.edu

*Deceased; this work is dedicated to his memory.

The mutual solubility and related liquid-liquid equilibria of C_7 hydrocarbons with water and heavy water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 23 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For 9 systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of the all experimental data for a given homologous series of aliphatic and aromatic hydrocarbons was used.
[DOI: 10.1063/1.1840737]

Key words: C_7 hydrocarbons; critical evaluation; heavy water; liquid-liquid equilibria; solubility; water

Contents

*A Critical Evaluation is prepared for this system.

List of Tables

List of Figures

1. Preface

1.1. Scope of this Volume

This paper is Part 5 of a revised and updated version of an earlier compilation and evaluation of the mutual solubilities of water and hydrocarbon compounds containing five or more carbon atoms.[1,2] This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

This revised work also includes all new evaluations for systems where two or more independent measurements of solubility have been reported. In these evaluations, reported solubility values are characterized as Recommended, Tentative, Doubtful, or Rejected, based on consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.[3–6] 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 (Maczynski and Shaw[7]) The derivation of the smoothing equations used to calculate reference values can be found in Parts 1 and 2 (Maczynski and Shaw[7,8]).

1.2. References for the Preface

[1] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 37, *Hydrocarbons with Water and Seawater, Part I: Hydrocarbons* 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 C_5-C_{11} 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: Binary Unsaturated Hydrocarbon—Water Systems, J. Phys. Chem. Ref. Data **33**, 579 (2004).

[6] M. Goral, A. Maczynski, and B. Wisniewska–Goclowska, Recommended Liquid-Liquid Equilibrium Data, Part 3: Binary Aromatic Hydrocarbon-Water System, J. Phys. Chem. Ref. Data **33**, 1159 (2004).

[7] A. Maczynski and D. Shaw, Editors, IUPAC-NIST Solubility Data Series. 81. Hydrocarbons 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_7 Hydrocarbons with Water and Heavy Water

2.1. 1,3,5-Cycloheptatriene+Water

Components:	**Evaluators:**
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

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

The experimental solubility data for (1) in (2) have been investigated by McAuliffe[2] at 298 K and Pierotti and Liabastre[3] at 278 K–318 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:

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

where $\ln x_{1,\min} = -9.09$, $\Delta_{\mathrm{sln}}\, C_p / R = 37.1$, and $T_{\min} = 298$ K.

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

The experimental and reference data of McAuliffe,[2] and Pierotti and Liabastre[3] are listed in Table 1. Since only one experimental data point is available at each temperature, no data can be Recommended. The data of McAuliffe[2] and Pierotti and Liabastre[2] in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

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

The experimental solubility data for (1) in (2) have been investigated by Englin *et al.*[1] at 303 K–323 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:

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

where: $d_1 = 0.489$, $d_2 = -1.227$, $d_3 = -1.196$, $d_4 = -8.963$, and $T_r = T/558.3$.

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-cycloheptatriene 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 2. All the data are in good agreement with the reference data and are Tentative.

References:

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

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

[3] R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).

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

T/K	Experimental values x_1 (T=tentative)	Reference values $x_1 \pm 30\%$
278.3	$1.136 \cdot 10^{-4}$ (T; Ref. 3)	$1.2 \cdot 10^{-4}$
288.4	$1.299 \cdot 10^{-4}$ (T; Ref. 3)	$1.2 \cdot 10^{-4}$
298.2	$1.21 \cdot 10^{-4}$ (T; Ref. 2)	$1.1 \cdot 10^{-4}$
298.3	$1.309 \cdot 10^{-4}$ (T; Ref. 3)	$1.1 \cdot 10^{-4}$
308.4	$1.45 \cdot 10^{-4}$ (T; Ref. 3)	$1.2 \cdot 10^{-4}$
318.4	$1.495 \cdot 10^{-4}$ (T; Ref. 3)	$1.2 \cdot 10^{-4}$

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

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
303.2	$3.21 \cdot 10^{-3}$ (T; Ref. 1)	$3.8 \cdot 10^{-3}$
313.2	$3.94 \cdot 10^{-3}$ (T; Ref. 1)	$4.9 \cdot 10^{-3}$
323.2	$5.06 \cdot 10^{-3}$ (T; Ref. 1)	$6.2 \cdot 10^{-3}$

Components:

(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2]
(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: 30 °C–50 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in 1,3,5-cycloheptatriene

$t/°C$	$10^3 \cdot x_2$ (compiler)	$g(2)/100$ g sln
30	3.21	0.0630
40	3.94	0.0773
50	5.06	0.0993

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Not specified
(2) Not specified.

Estimated Error:

Not specified.

Components:

(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2]
(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 1,3,5-cycloheptatriene in water at 25 °C was reported to be 620 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0620 $g(1)/100$ g sln and $1.21 \cdot 10^{-4}$.

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 conjunction 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: 20 mg (1)/kg (2) (standard deviation of mean).

Components:	**Original Measurements:**
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (2) Water; H_2O; [7732-18-5]	R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).
Variables:	**Prepared By:**
Temperature: 278.26 K–318.36 K	M. C. Haulait-Pirson

Experimental Data

Solubility of 1,3,5-cycloheptatriene in water

T/K	$10^3 \cdot x_1$	$g(1)$/100 g sln
278.26	0.1136	0.05809±0.0014
288.36	0.1299	0.06645±0.0017
298.26	0.1309	0.06694±0.0019
308.36	0.1450	0.07418±0.0019
318.36	0.1495	0.07648±0.0022

Auxiliary Information

Method/Apparatus/Procedure:

10 mL of (2) were placed along with 4–10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 h. The bottles were then hand shaken to remove (1) droplets from the stoppers and replaced in the bath with the tops down for an additional 24 h. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.

Source and Purity of Materials:

(1) Columbia Organic Chemicals Co., Inc.; Tech. 83%; used as received.
(2) Laboratory distilled water.

Estimated Error:

Solubility: standard deviation from at least 15 measurements are given above.

2.2. 1,6-Heptadiyne+Water

Components:	**Original Measurements:**
(1) 1,6-Heptadiyne; C_7H_8; [2396-63-6] (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 1,6-heptadiyne in water at 25 °C was reported to be 1650 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.1650 $g(1)$/100 g sln and $3.23 \cdot 10^{-4}$.

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. 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 conjunction 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: 25 mg (1)/kg (2) (standard deviation of the mean).

2.3. 2,5-Norbornadiene+Water

Components:

(1) 2,5-Norbornadiene; C_7H_8; [121-46-0]
(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–50 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in 2,5-norbornadiene

$t/°C$	$10^3 \cdot x_2$ (compiler)	$g(2)/100$ g sln
20	1.51	0.0295
30	1.96	0.0383
50	3.44	0.0675

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.

2.4. Toluene+Water

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Evaluators:

A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, September, 2003.

Critical Evaluation of the Solubility of Toluene (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
Anderson and Prausnitz[1]	373–474 (153–2363 kPa)	Mackay and Shiu[38]	298
Andrews and Keefer[2]	298	McAuliffe[39]	298
Banerjee[3]	298	McAuliffe[40]	298
Banerjee *et al.*[4]	298	Miller and Hawthorne[41]	298–473 (5000 kPa)
Ben-Naim and Wilf[5]	283–293	Morrison and Billett[42]	298
Ben-Naim and Wilf[6]	298	Pierotti and Liabastre[44]	278–318
Bohon and Claussen[8]	298	Polak and Lu[45]	273–298
Booth and Everson[9]	298	Price[46]	298
Bradley *et al.*[10]	298–328	Rossi and Thomas[48]	298
Brown *et al.*[11]	341–524 (6800 kPa)	Sada *et al.*[49]	298
Brown and Wasik[12]	278–293	Sanemasa *et al.*[50]	298
Chandler *et al.*[14]	473–548 (2500–8600 kPa)	Sanemasa *et al.*[51]	288–318
Chen and Wagner[15]	303–373 (100–350 kPa)	Sanemasa *et al.*[52]	288–318
Chey and Calder[16]	294	Sanemasa *et al.*[53]	298
Dohanyosova *et al.*[18]	274–328	Sawamura *et al.*[54]	298 (100 kPa)
Fühner[20]	289	Sawamura *et al.*[55]	273–323
Gross and Saylor[23]	303	Schwarz[56]	297
Guseva and Parnov[24]	360–480	Schwarz and Miller[57]	283–303
Guseva and Parnov[25]	363–497	Stephenson[58]	273–363
Keeley *et al.*[31]	298	Sutton and Calder[59]	298
Klevens[32]	298	Tamura *et al.*[60]	298
Korenman and Aref'eva[33]	293	Tewari *et al.*[62]	298
Korenman and Aref'eva[34]	298	Uspenskii[63]	283–295
Krasnoshchekova and Gubergrits[35]	298	Vesala[64]	298
Lo *et al.*[36]	298	Wing and Johnston[65]	298
Ma *et al.*[37]	278–318		

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 $\ln x_{\min,1} = -9.14$, $D = 35.7$, 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 the Table 3.

All the experimental and reference data are listed in the Table 4 and shown in Fig. 1. The Recommended and Tentative data are shown in Fig. 2.

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

The experimental solubility data for (2) in (1) 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
Anderson and Prausnitz[1]	373–474 (153–2363 kPa)	Johnson *et al.*[29]	298
Benkovski *et al.*[7]	303	Jones and Monk[30]	298–308
Brown *et al.*[11]	422–524 (6800 kPa)	Peschke and Sandler[43]	298
Caddock and Davies[13]	293	Polak and Lu[45]	273–298
Chen and Wagner[15]	303–373 (100–350 kPa)	Rosenbaum and Walton[47]	283–323
Chandler *et al.*[14]	473–548 (2500–8600 kPa)	Stephenson[58]	273–363
Englin *et al.*[19]	273–323	Tamura *et al.*[60]	298
Glasoe and Schultz[21]	288–303	Tarassenkow and Poloshinzewa[61]	264–366
Gregory *et al.*[22]	298	Uspenskii[63]	283–295
Högfeldt and Bolander[27]	298		

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

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

where $d_1 = -0.495$, $d_2 = -3.700$, $d_3 = -0.102$, $d_4 = -4.641$, and $T_r = T/553.0$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of toluene in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 5.

The experimental and reference solubility data for (2) in (1) are listed in Table 6 and shown in Fig. 3. The Recommended and Tentative data are shown in Fig. 4.

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

The experimental high pressure solubility for (1) in (2) investigated by the authors listed below have not been critically evaluated because the developed method is not applied for such data. An evaluation of these data was presented by Hefter and Young.[71]

Author (s)	T/K	Author (s)	T/K
Bradley *et al.*[10]	298–328 (100 000 kPa)	Haruki *et al.*[26]	573 (10 500–28 100 kPa)
Chandler *et al.*[14]	523–548 (17 200 kPa)	Jäger[28]	423–573
Connolly[17]	553–583 (14 700–60 800 kPa)	Sawamura *et al.*[54]	298 (25 000–400 000 kPa)

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[68] are independent data. The data reported by Alwani and Schneider,[66] Gill *et al.*,[67] Roof,[69] Tarassenkov and Polozhinzeva,[70] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1] F. E. Anderson and J. M. Prausnitz, Fluid Phase Equilib. **32**, 63 (1986).
[2] L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[3] S. Banerjee, Environ. Sci. Technol. **18**, 587 (1984).
[4] S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
[5] A. Ben-Naim and J. Wilf, J. Chem. Phys. **70**, 771 (1979).
[6] A. Ben-Naim and J. Wilf, J. Phys. Chem. **84**, 583 (1980).
[7] V. G. Benkovski, M. H. Nauruzov, and T. M. Bogoslovskaya, Tr. Inst. Khim. Nefti Prir. Solei, Akad. Nauk Kaz. SSR **2**, 25.
[8] R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
[9] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
[10] R. S. Bradley, M. J. Dew, and D. C. Munro, High Temperature:- High Pressures **5**, 169 (1973).
[11] J. S. Brown, J. P. Hallett, D. Bush, and C. A. Eckert, J. Chem. Eng. Data **45**, 846 (2000).
[12] R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A **78**, 453 (1974).
[13] B. D. Caddock and P. L. Davies, J. Inst. Pet. **46**, 391 (1960).
[14] K. Chandler, B. Eason, C. L. Liotta, and C. A. Eckert, Ind. Eng. Chem. Res. **37**, 3515 (1998).
[15] H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 475 (1994).
[16] W. Chey and G. V. Calder, J. Chem. Eng. Data **17**, 199 (1972).
[17] J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).
[18] P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001).
[19] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[20] H. Führer, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).
[21] P. K. Glasoe and S. D. Schultz, J. Chem. Eng. Data **17**, 66 (1972).
[22] M. D. Gregory, S. D. Christian, and H. E. Affsprung, J. Phys. Chem. **71**, 2283 (1967).
[23] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
[24] A. N. Guseva and E. I. Parnov, Radiokhimiya **5**, 507 (1963).
[25] A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. **18**, 76 (1963).
[26] M. Haruki, Y. Iwai, S. Nagao, and Y. Arai, J. Chem. Eng. Data **46**, 950 (2001).
[27] E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).
[28] A. Jäger, Brennst.-Chem. **4**, 259 (1923).
[29] J. R. Johnson, S. D. Christian, and H. E. Affsprung, J. Chem. Soc. A **77** (1966).
[30] J. R. Jones and C. B. Monk, J. Chem. Soc. 2633 (1963).
[31] D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **33**, 87 (1988).
[32] H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[33] I. M. Korenman and R. P. Aref'eva, Patent USSR 553 524, 1977.04.05.
[34] I. M. Korenman and R. P. Aref'eva, Zh. Prikl. Khim. (Leningrad) **51**, 957 (1978).
[35] R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy **2**, 170 (1975).
[36] J. M. Lo, C. L. Tseng, and J. Y. Yang, Anal. Chem. **58**, 1596 (1986).
[37] J. H. Y. Ma, H. Hung, W.-Y. Shiu, and D. Mackay, J. Chem. Eng. Data **46**, 619 (2001).
[38] D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).
[39] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[40] C. McAuliffe, Nature (London) **200**, 1092 (1963).
[41] D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).
[42] T. J. Morrison and F. Billett, J. Chem. Soc. 3819 (1952).
[43] N. Peschke and S. I. Sandler, J. Chem. Eng. Data **40**, 315 (1995).
[44] R. A. Pierotti and A. A. Liabastre, U.S. NITS, PB Rep. No 21163, 113 pp (1972).
[45] J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[46] L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[47] C. K. Rosenbaum and J. H. Walton, J. Am. Chem. Soc. **52**, 3568 (1930).
[48] S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).
[49] E. Sada, S. Kito, and Y. Ito, J. Chem. Eng. Data **20**, 373 (1975).
[50] I. Sanemasa, S. Arakawa, M. Araki, and T. Deguchi, Bull. Chem. Soc. Jpn. **57**, 1539 (1984).
[51] I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[52] I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).
[53] I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).
[54] S. Sawamura, K. Kitamura, and Y. Taniguchi, J. Phys. Chem. **93**, 4931 (1989).
[55] S. Sawamura, K. Nagaoka, and T. Machikawa, J. Phys. Chem. **105**, 2429 (2001).
[56] F. P. Schwarz, Anal. Chem. **52**, 10 (1980).
[57] F. P. Schwarz and J. Miller, Anal. Chem. **52**, 2162 (1980).
[58] R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).
[59] C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[60] K. Tamura, Y. Chen, and T. Yamada, J. Chem. Eng. Data **46**, 1381 (2001).
[61] D. N. Tarassenkow and E. N. Poloshinzewa, Ber. Dtsch. Chem. Ges. **65**, 184 (1932).
[62] Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[63] S. P. Uspenskii, Neft. Khoz. **11–12**, 713 (1929).
[64] A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).
[65] J. Wing and W. H. Johnston, J. Am. Chem. Soc. **79**, 864 (1957).
[66] Z. Alwani and G. Schneider, Ber. Bunsenges. Phys. Chem. **71**, 633 (1967).
[67] S. J. Gill, N. F. Nichols, and I. Wadso, J. Chem. Thermodyn. **8**, 445 (1976).
[68] T. Krzyzanowski and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).
[69] J. G. Roof, J. Chem. Eng. Data **15**, 301 (1970).
[70] D. N. Tarassenkov and E. N. Polozhinzeva, Zh. Obshch. Khim. **1**, 71 (1931).
[71] D. Shaw, Editor, IUPAC Solubility Data Series Volume 37, *Hydrocarbons with Water and Seawater, Part 1: Hydrocarbon*, C_5 *to* C_7 (Pergamon, New York, 1989).

TABLE 3. The data categories for solubility of toluene (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		Polak and Lu[45] Sawamura *et al.*[55]	Stephenson[58]
273.7		Dohanyosova *et al.*[18]	
277.7		Brown and Wasik[12]	
278.2	Dohanyosova *et al.*[18] Ma *et al.*[37] Pierotti and Liabastre[44] Sawamura *et al.*[55]		
279.5		Brown and Wasik[12]	
280.3		Brown and Wasik[12]	
282.2		Brown and Wasik[12]	
282.7			Stephenson[58]
283.1		Pierotti and Liabastre[44]	
283.2	Ben-Naim and Wilf[5] Sawamura *et al.*[55]		Schwarz and Miller[57] Uspenskii[63]
285.0		Brown and Wasik[12]	
285.3		Brown and Wasik[12]	
288.2	Dohanyosova *et al.*[18] Ma *et al.*[37] Sanemasa *et al.*[51] Sanemasa *et al.*[52] Sawamura *et al.*[55]		
288.3		Brown and Wasik[12]	
289.2		Führer[20]	
291.1		Brown and Wasik[12]	
293.0			Stephenson[58]
293.1		Pierotti and Liabastre[44]	
293.2	Ben-Naim and Wilf[5] Korenman and Aref'eva[33] Sawamura *et al.*[55]		Schwarz and Miller[57]
293.3		Brown and Wasik[12]	
294.0		Chey and Calder[16]	
295.2		Uspenskii[63]	
296.6	Schwarz[56]		
298.0	Miller and Hawthorne[41] Vesala[64]		
298.1		Sanemasa *et al.*[53]	
298.2	Andrews and Keefer[2] Banerjee[3] Ben-Naim and Wilf[6] Bohon and Claussen[8] Bradley *et al.*[10] Dohanyosova *et al.*[18] Keeley *et al.*[31] Lo *et al.*[36] Ma *et al.*[37] Mackay and Shiu[38] McAuliffe[39] McAuliffe[40] Morrison and Billett[42] Pierotti and Liabastre[44] Polak and Lu[45] Price[46] Sanemasa *et al.*[50] Sanemasa *et al.*[51] Sanemasa *et al.*[52] Sanemasa *et al.*[53] Sawamura *et al.*[54] Sawamura *et al.*[55] Stephenson[58] Sutton and Calder[59] Tamura *et al.*[60] Tewari *et al.*[62]	Klevens[32] Korenman and Aref'eva[34] Sada *et al.*[49]	Banerjee *et al.*[4] Booth and Everson[9] Krasnoshchekova and Gubergrits[35] Rossi and Thomas[48] Wing and Johnston[65]
302.9			Stephenson[58]
303.2	Chen and Wagner[15] Gross and Saylor[23] Sawamura *et al.*[55]		Schwarz and Miller[57]
308.2	Dohanyosova *et al.*[18] Ma *et al.*[37] Sanemasa *et al.*[51] Sanemasa *et al.*[52] Sawamura *et al.*[55]		
308.3		Pierotti and Liabastre[44]	
312.8			Stephenson[58]
313.2	Chen and Wagner[15] Sawamura *et al.*[55] Stephenson[58]		
318.2	Dohanyosova *et al.*[18] Ma *et al.*[37] Sanemasa *et al.*[51] Sanemasa *et al.*[52] Sawamura *et al.*[55]	Bradley *et al.*[10]	
318.5		Pierotti and Liabastre[44]	
323.0		Miller and Hawthorne[41]	
323.2	Chen and Wagner[15] Sawamura *et al.*[55]		Stephenson[58]
328.2		Bradley *et al.*[10] Dohanyosova *et al.*[18]	
333.2		Chen and Wagner[15]	
333.3			Stephenson[58]
340.6		Brown *et al.*[11]	
343.2		Chen and Wagner[15]	
343.6		Stephenson[58]	

353.2	Chen and Wagner[15]	
354.2	Stephenson[58]	
360.2		Guseva and Parnov[24]
363.2	Chen and Wagner[15]	Guseva and Parnov[24]
363.4	Stephenson[58]	
372.6	Anderson and Prausnitz[1]	
373.0	Miller and Hawthorne[41]	
373.2	Chen and Wagner[15]	
384.1	Brown *et al.*[11]	
387.2		Guseva and Parnov[24,25]
396.2		Guseva and Parnov[24]
398.0	Anderson and Prausnitz[1]	
403.2	Brown *et al.*[11]	
417.2	Brown *et al.*[11]	
420.2		Guseva and Parnov[24,25]
422.6	Anderson and Prausnitz[1]	
423.0	Miller and Hawthorne[41]	
437.7		Guseva and Parnov[24]
442.2		Guseva and Parnov[24,25]
445.0	Brown *et al.*[11]	
448.4	Anderson and Prausnitz[1]	
448.5	Anderson and Prausnitz[1]	
456.2		Guseva and Parnov[25]
473.0	Miller and Hawthorne[41]	
473.2	Chandler *et al.*[14]	
473.6	Anderson and Prausnitz[1]	
476.2		Guseva and Parnov[24]
480.2		Guseva and Parnov[24,25]
485.2	Brown *et al.*[11]	
497.2		Guseva and Parnov[25]
518.0	Brown *et al.*[11]	
523.2	Chandler *et al.*[14]	
548.2	Chandler *et al.*[14]	

TABLE 4. Experimental values for solubility of toluene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2		$1.42\cdot10^{-4}$ (T; Ref. 45), $1.14\cdot10^{-4}$ (T; Ref. 55), $2.30\cdot10^{-4}$ (D; Ref. 58)	$1.2\cdot10^{-4}$
273.7		$1.10\cdot10^{-4}$ (T; Ref. 18)	$1.1\cdot10^{-4}$
277.7		$1.20\cdot10^{-4}$ (T; Ref. 12)	$1.1\cdot10^{-4}$
278.2		$1.08\cdot10^{-4}$ (R; Ref. 18), $1.06\cdot10^{-4}$ (R; Ref. 37), $1.243\cdot10^{-4}$ (R; Ref. 44), $1.111\cdot10^{-4}$ (R; Ref. 55)	$1.1\cdot10^{-4}$
279.5		$1.18\cdot10^{-4}$ (T; Ref. 12)	$1.1\cdot10^{-4}$
280.3		$1.15\cdot10^{-4}$ (T; Ref. 12)	$1.1\cdot10^{-4}$
282.2		$1.15\cdot10^{-4}$ (T; Ref. 12)	$1.1\cdot10^{-4}$
282.7		$1.80\cdot10^{-4}$ (D; Ref. 58)	$1.1\cdot10^{-4}$
283.1		$1.236\cdot10^{-4}$ (T; Ref. 44)	$1.1\cdot10^{-4}$
283.2		$1.119\cdot10^{-4}$ (R; Ref. 5), $1.09\cdot10^{-4}$ (R; Ref. 55), $1.483\cdot10^{-4}$ (D; Ref. 57), $1.52\cdot10^{-4}$ (D; Ref. 57), $7.20\cdot10^{-5}$ (D; Ref. 63)	$1.1\cdot10^{-4}$
285.0		$1.12\cdot10^{-4}$ (T; Ref. 12)	$1.1\cdot10^{-4}$
285.3		$1.13\cdot10^{-4}$ (T; Ref. 12)	$1.1\cdot10^{-4}$
288.2		$1.06\cdot10^{-4}$ (R; Ref. 18), $1.01\cdot10^{-4}$ (R; Ref. 37), $1.01\cdot10^{-4}$ (R; Ref. 51), $1.04\cdot10^{-4}$ (R; Ref. 52), $1.08\cdot10^{-4}$ (R; Ref. 55)	$1.1\cdot10^{-4}$
288.3		$1.11\cdot10^{-4}$ (T; Ref. 12)	
289.2		$9.20\cdot10^{-5}$ (T; Ref. 20)	$1.1\cdot10^{-4}$
291.1		$1.13\cdot10^{-4}$ (T; Ref. 12)	$1.1\cdot10^{-4}$
293.0		$1.60\cdot10^{-4}$ (D; Ref. 58)	$1.1\cdot10^{-4}$
293.1		$1.292\cdot10^{-4}$ (T; Ref. 53)	
293.2		$1.15\cdot10^{-4}$ (R; Ref. 5), $1.11\cdot10^{-4}$ (R; Ref. 33), $1.08\cdot10^{-4}$ (R; Ref. 55), $1.43\cdot10^{-4}$ (D; Ref. 57), $1.45\cdot10^{-4}$ (D; Ref. 57)	$1.1\cdot10^{-4}$
293.3		$1.11\cdot10^{-4}$ (T; Ref. 12),	$1.1\cdot10^{-4}$
294.0		$9.36\cdot10^{-5}$ (T; Ref. 16)	$1.1\cdot10^{-4}$
295.2		$9.62\cdot10^{-5}$ (T; Ref. 63)	$1.1\cdot10^{-4}$
296.6		$1.31\cdot10^{-4}$ (R; Ref. 56), $1.29\cdot10^{-4}$ (R; Ref. 56)	$1.1\cdot10^{-4}$
298.0	5000 (Ref. 41)	$1.07\cdot10^{-4}$ (T; Ref. 41), $1.226\cdot10^{-4}$ (T; Ref. 64)	$1.1\cdot10^{-4}$
298.1		$1.021\cdot10^{-4}$ (T; Ref. 53)	$1.1\cdot10^{-4}$
298.2	100 (Ref. 10) 100 (Ref. 54)	$1.04\cdot10^{-4}$ (R; Ref. 2), $1.027\cdot10^{-4}$ (R; Ref. 3), $3.04\cdot10^{-4}$ (D; Ref. 4), $1.209\cdot10^{-4}$ (R; Ref. 6), $1.23\cdot10^{-4}$ (R; Ref. 8), $6.80\cdot10^{-5}$ (D; Ref. 9), $1.07\cdot10^{-4}$ (R; Ref. 10), $1.09\cdot10^{-4}$ (R; Ref. 18), $1.13\cdot10^{-4}$ (R; Ref. 31), $9.80\cdot10^{-5}$ (T; Ref. 32), $1.27\cdot10^{-4}$ (T; Ref. 34), $4.30\cdot10^{-5}$ (D; Ref. 35), $1.02\cdot10^{-4}$ (R; Ref. 36), $1.02\cdot10^{-4}$ (R; Ref. 37), $1.015\cdot10^{-4}$ (R; Ref. 38), $1.01\cdot10^{-4}$ (R; Ref. 39), $1.05\cdot10^{-4}$ (R; Ref. 40), $1.05\cdot10^{-4}$ (R; Ref. 42), $1.232\cdot10^{-4}$ (R; Ref. 44), $1.12\cdot10^{-4}$ (R; Ref. 45), $1.08\cdot10^{-4}$ (R; Ref. 46), $5.50\cdot10^{-6}$ (D; Ref. 48), $9.58\cdot10^{-5}$ (T; Ref. 49), $1.02\cdot10^{-4}$ (R; Ref. 50), $1.03\cdot10^{-4}$ (R; Ref. 51), $1.09\cdot10^{-4}$ (R; Ref. 52), $1.021\cdot10^{-4}$ (R; Ref. 53), $1.10\cdot10^{-4}$ (R; Ref. 54), $1.09\cdot10^{-4}$ (R; Ref. 55), $1.04\cdot10^{-4}$ (R; Ref. 58), $1.046\cdot10^{-4}$ (R; Ref. 59), $1.00\cdot10^{-4}$ (R; Ref. 60), $1.135\cdot10^{-4}$ (R; Ref. 62), $5.70\cdot10^{-5}$ (D; Ref. 65)	$1.1\cdot10^{-4}$
302.9		$1.60\cdot10^{-4}$ (D; Ref. 58)	$1.1\cdot10^{-4}$
303.2	100 (Ref. 15)	$1.17\cdot10^{-4}$ (R; Ref. 15), $1.12\cdot10^{-4}$ (R; Ref. 23), $1.121\cdot10^{-4}$ (R; Ref. 55), $1.80\cdot10^{-4}$ (D; Ref. 57), $1.475\cdot10^{-4}$ (D; Ref. 57)	$1.1\cdot10^{-4}$

308.2		$1.16\cdot10^{-4}$ (R; Ref. 18), $1.09\cdot10^{-4}$ (R; Ref. 37), $1.07\cdot10^{-4}$ (R; Ref. 51), $1.16\cdot10^{-4}$ (R; Ref. 52), $1.151\cdot10^{-4}$ (R; Ref. 55)	$1.1\cdot10^{-4}$
308.3		$1.314\cdot10^{-4}$ (T; Ref. 44)	$1.1\cdot10^{-4}$
312.8		$2.00\cdot10^{-4}$ (D; Ref. 58)	$1.2\cdot10^{-4}$
313.2	100 (Ref. 15)	$1.19\cdot10^{-4}$ (R; Ref. 15), $1.201\cdot10^{-4}$ (R; Ref. 55), $1.20\cdot10^{-4}$ (R; Ref. 58)	$1.2\cdot10^{-4}$
318.2	100 (Ref. 10)	$1.41\cdot10^{-4}$ (T; Ref. 10), $1.25\cdot10^{-4}$ (R; Ref. 18), $1.25\cdot10^{-4}$ (R; Ref. 37), $1.14\cdot10^{-4}$ (R; Ref. 51), $1.25\cdot10^{-4}$ (R; Ref. 52), $1.251\cdot10^{-4}$ (R; Ref. 55)	$1.2\cdot10^{-4}$
318.5		$1.313\cdot10^{-4}$ (T; Ref. 44)	$1.2\cdot10^{-4}$
323.0	5000 (Ref. 41)	$1.25\cdot10^{-4}$ (T; Ref. 41)	$1.3\cdot10^{-4}$
323.2	100 (Ref. 15)	$1.27\cdot10^{-4}$ (R; Ref. 15), $1.322\cdot10^{-4}$ (R; Ref. 55), $1.80\cdot10^{-4}$ (D; Ref. 58)	$1.3\cdot10^{-4}$
328.2	100 (Ref. 10)	$1.68\cdot10^{-4}$ (T; Ref. 10), $1.40\cdot10^{-4}$ (T; Ref. 18)	$1.4\cdot10^{-4}$
333.2	150 (Ref. 15)	$1.44\cdot10^{-4}$ (T; Ref. 15)	$1.5\cdot10^{-4}$
333.3		$2.00\cdot10^{-4}$ (D; Ref. 58)	$1.5\cdot10^{-4}$
340.6	6800 (Ref. 11)	$1.83\cdot10^{-4}$ (T; Ref. 11)	$1.6\cdot10^{-4}$
343.2	250 (Ref. 15)	$1.71\cdot10^{-4}$ (T; Ref. 15)	$1.7\cdot10^{-4}$
343.6		$1.80\cdot10^{-4}$ (T; Ref. 58)	$1.7\cdot10^{-4}$
353.2	250 (Ref. 15)	$1.98\cdot10^{-4}$ (T; Ref. 15)	$2.0\cdot10^{-4}$
354.2		$2.50\cdot10^{-4}$ (T; Ref. 58)	$2.0\cdot10^{-4}$
360.2		$6.82\cdot10^{-4}$ (D; Ref. 24)	$2.2\cdot10^{-4}$
363.2	350 (Ref. 15)	$2.32\cdot10^{-4}$ (T; Ref. 15), $8.30\cdot10^{-4}$ (D; Ref. 24)	$2.3\cdot10^{-4}$
363.4		$2.30\cdot10^{-4}$ (T; Ref. 58)	$2.3\cdot10^{-4}$
372.6	153 (Ref. 1)	$2.86\cdot10^{-4}$ (T; Ref. 1)	$2.8\cdot10^{-4}$
373.0	5000 (Ref. 41)	$2.70\cdot10^{-4}$ (T; Ref. 41)	$2.8\cdot10^{-4}$
373.2	350 (Ref. 15)	$1.68\cdot10^{-4}$ (T; Ref. 15)	$2.8\cdot10^{-4}$
384.1	6800 (Ref. 11)	$3.60\cdot10^{-4}$ (T; Ref. 11)	$3.5\cdot10^{-4}$
387.2		$1.59\cdot10^{-3}$ (D; Ref. 24), $1.619\cdot10^{-3}$ (D; Ref. 25)	$3.7\cdot10^{-4}$
396.2		$1.81\cdot10^{-3}$ (D; Ref. 24)	$4.4\cdot10^{-4}$
398.0	384 (Ref. 1)	$4.63\cdot10^{-4}$ (T; Ref. 1)	$4.6\cdot10^{-4}$
403.2	6800 (Ref. 11)	$5.27\cdot10^{-4}$ (T; Ref. 11)	$5.1\cdot10^{-4}$
417.2	6800 (Ref. 11)	$6.93\cdot10^{-4}$ (T; Ref. 11)	$6.9\cdot10^{-4}$
420.2		$3.21\cdot10^{-3}$ (D; Ref. 24), $3.248\cdot10^{-3}$ (D; Ref. 25)	$7.3\cdot10^{-4}$
422.6	753 (Ref. 1)	$7.94\cdot10^{-4}$ (T; Ref. 1)	$7.7\cdot10^{-4}$
423.0	5000 (Ref. 41)	$6.60\cdot10^{-4}$ (T; Ref. 41)	$7.8\cdot10^{-4}$
437.7		$4.22\cdot10^{-3}$ (D; Ref. 24)	$1.1\cdot10^{-3}$
442.2		$4.53\cdot10^{-3}$ (D; Ref. 24), $4.737\cdot10^{-3}$ (D; Ref. 25)	$1.2\cdot10^{-3}$
445.0	6800 (Ref. 11)	$1.18\cdot10^{-3}$ (T; Ref. 11)	$1.3\cdot10^{-3}$
448.4	1425(Ref. 1)	$1.30\cdot10^{-3}$ (T; Ref. 1)	$1.4\cdot10^{-3}$
448.5	1404 (Ref. 1)	$1.23\cdot10^{-3}$ (T; Ref. 1)	$1.4\cdot10^{-3}$
456.2		$5.579\cdot10^{-3}$ (D; Ref. 25)	$1.6\cdot10^{-3}$
473.0	5000 (Ref. 41)	$1.90\cdot10^{-3}$ (T; Ref. 41)	$2.4\cdot10^{-3}$
473.2	2500 (Ref. 14)	$2.38\cdot10^{-3}$ (T; Ref. 14)	$2.4\cdot10^{-3}$
473.6	2363 (Ref. 1)	$2.59\cdot10^{-3}$ (T; Ref. 1)	$2.4\cdot10^{-3}$
476.2		$7.51\cdot10^{-3}$ (D; Ref. 24)	$2.6\cdot10^{-3}$
480.2		$7.96\cdot10^{-3}$ (D; Ref. 24), $8.314\cdot10^{-3}$ (D; Ref. 25)	
485.2	6800 (Ref. 11)	$2.68\cdot10^{-3}$ (T; Ref. 11)	$3.1\cdot10^{-3}$
497.2		$1.0336\cdot10^{-2}$ (D; Ref. 25)	$4.1\cdot10^{-4}$
518.0	6800 (Ref. 11)	$5.47\cdot10^{-3}$ (T; Ref. 11)	$6.6\cdot10^{-3}$
523.2	5800 (Ref. 14)	$7.03\cdot10^{-3}$ (T; Ref. 14)	$7.4\cdot10^{-3}$
548.2	8600 (Ref. 14)	$1.29\cdot10^{-2}$ (T; Ref. 14)	$1.3\cdot10^{-3}$

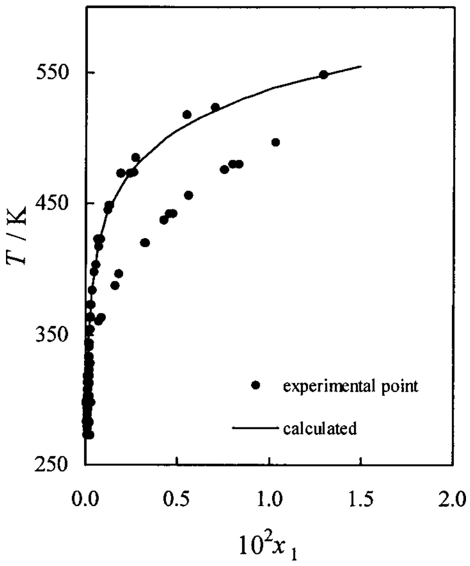

FIG. 1. All the solubility data for toluene (1) in water (2).

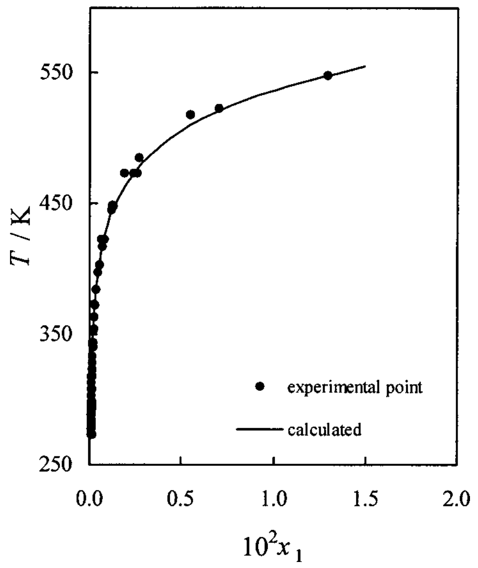

FIG. 2. Recommended and tentative solubility data for toluene (1) in water (2).

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

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)
264.2			Tarassenkow and Poloshinzewa[61]
269.7			Tarassenkow and Poloshinzewa[61]
273.2		Englin *et al.*[19] Polak and Lu[45]	Stephenson[58]
282.7			Stephenson[58]
283.2	Englin *et al.*[19] Rosenbaum and Walton[47]	Uspenskii[63]	
283.7			Tarassenkow and Poloshinzewa[61]
288.2		Glasoe and Schultz[21]	
291.2		Tarassenkow and Poloshinzewa[61]	
293.0			Stephenson[58]
293.2	Caddock and Davies[13] Englin *et al.*[19] Rosenbaum and Walton[47]		
295.2		Uspenskii[63]	
298.2	Glasoe and Schultz[21] Gregory *et al.*[22] Högfeldt and Bolander[27] Johnson *et al.*[29] Polak and Lu[45]	Jones and Monk[30] Peschke and Sandler[43] Stephenson[58]	Glasoe and Schultz[21] Tamura *et al.*[60]
302.9			Stephenson[58]
303.0		Benkovski *et al.*[7]	
303.2	Englin *et al.*[19] Glasoe and Schultz[21]	Chen and Wagner[15] Glasoe and Schultz[21] Jones and Monk[30] Rosenbaum and Walton[47] Tarassenkow and Poloshinzewa[61]	
308.2		Jones and Monk[30]	
311.7		Tarassenkow and Poloshinzewa[61]	
312.8		Stephenson[58]	
313.2		Chen and Wagner[15] Englin *et al.*[19] Rosenbaum and Walton[47] Stephenson[58]	
321.2		Tarassenkow and Poloshinzewa[61]	
323.2		Chen and Wagner[15] Englin *et al.*[19] Rosenbaum and Walton[47] Stephenson[58]	
333.2		Chen and Wagner[15]	
333.3		Stephenson[58]	
333.7		Tarassenkow and Poloshinzewa[61]	
341.2		Tarassenkow and Poloshinzewa[61]	
343.2		Chen and Wagner[15]	
343.6		Stephenson[58]	
349.2		Tarassenkow and Poloshinzewa[61]	
353.2		Chen and Wagner[15]	
354.2		Stephenson[58]	
357.2		Tarassenkow and Poloshinzewa[61]	
363.2		Chen and Wagner[15]	
363.4		Stephenson[58]	
366.2		Tarassenkow and Poloshinzewa[61]	
372.6		Anderson and Prausnitz[1]	
373.2		Chen and Wagner[15]	
398.0		Anderson and Prausnitz[1]	

422.6	Anderson and Prausnitz[1]
422.8	Brown *et al.*[11]
429.2	Brown *et al.*[11]
448.4	Anderson and Prausnitz[1]
448.5	Anderson and Prausnitz[1]
451.1	Brown *et al.*[11]
453.3	Brown *et al.*[11]
467.8	Brown *et al.*[11]
470.9	Brown *et al.*[11]
473.2	Chandler *et al.*[14]
473.6	Anderson and Prausnitz[1]
479.8	Brown *et al.*[11]
485.1	Brown *et al.*[11]
488.4	Brown *et al.*[11]
494.7	Brown *et al.*[11]
502.5	Brown *et al.*[11]
504.2	Brown *et al.*[11]
513.5	Brown *et al.*[11]
521.6	Brown *et al.*[11]
523.2	Chandler *et al.*[14]
524.3	Brown *et al.*[11]
548.2	Chandler *et al.*[14]

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

T/K	P/kPa	Experimental values x_2 (R = recommended, T = tentative, D = doubtful)	Reference values $x_2 \pm 30\%$
264.2		$1.00\cdot 10^{-4}$ (D; Ref. 61)	$8.7\cdot 10^{-4}$
269.7		$3.00\cdot 10^{-4}$ (D; Ref. 61)	$1.1\cdot 10^{-3}$
273.2		$1.382\cdot 10^{-3}$ (T; Ref. 19), $1.17\cdot 10^{-3}$ (T; Ref. 45), $2.14\cdot 10^{-3}$ (D; Ref. 58)	$1.2\cdot 10^{-3}$
282.7		$2.91\cdot 10^{-3}$ (D; Ref. 58)	$1.7\cdot 10^{-3}$
283.2		$1.61\cdot 10^{-3}$ (R; Ref. 19), $1.71\cdot 10^{-3}$ (R; Ref. 47), $2.18\cdot 10^{-3}$ (T; Ref. 63)	$1.7\cdot 10^{-3}$
283.7		$1.00\cdot 10^{-3}$ (D; Ref. 61)	$1.7\cdot 10^{-3}$
288.2		$2.11\cdot 10^{-3}$ (T; Ref. 21), $1.71\cdot 10^{-3}$ (T; Ref. 21)	$2.0\cdot 10^{-3}$
291.2		$1.70\cdot 10^{-3}$ (T; Ref. 61)	$2.2\cdot 10^{-3}$
293.0		$4.43\cdot 10^{-3}$ (D; Ref. 58)	$2.4\cdot 10^{-3}$
293.2		$2.30\cdot 10^{-3}$ (R; Ref. 13), $2.35\cdot 10^{-3}$ (R; Ref. 19), $2.30\cdot 10^{-3}$ (R; Ref. 47)	$2.4\cdot 10^{-3}$
295.2		$2.68\cdot 10^{-3}$ (T; Ref. 63)	$2.6\cdot 10^{-3}$
298.2		$2.78\cdot 10^{-3}$ (R; Ref. 21), $5.04\cdot 10^{-2}$ (D; Ref. 21), $2.86\cdot 10^{-3}$ (R; Ref. 22), $2.80\cdot 10^{-3}$ (R; Ref. 27), $2.92\cdot 10^{-3}$ (R; Ref. 29), $2.40\cdot 10^{-3}$ (T; Ref. 30), $2.30\cdot 10^{-3}$ (T; Ref. 43), $2.77\cdot 10^{-3}$ (R; Ref. 45), $3.06\cdot 10^{-3}$ (T; Ref. 58), $4.70\cdot 10^{-3}$ (D; Ref. 60)	$2.8\cdot 10^{-3}$
302.9		$4.69\cdot 10^{-3}$ (D; Ref. 58)	$3.2\cdot 10^{-3}$
303.0		$7.39\cdot 10^{-2}$ (T; Ref. 7)	$3.2\cdot 10^{-3}$
303.2	100 (Ref. 15)	$2.91\cdot 10^{-3}$ (T; Ref. 15), $3.14\cdot 10^{-3}$ (R; Ref. 19), $3.14\cdot 10^{-3}$ (R; Ref. 21), $5.60\cdot 10^{-2}$ (T; Ref. 21), $2.80\cdot 10^{-3}$ (T; Ref. 30), $3.06\cdot 10^{-3}$ (T; Ref. 47), $2.70\cdot 10^{-3}$ (T; Ref. 61)	$3.3\cdot 10^{-3}$
308.2		$3.50\cdot 10^{-3}$ (T; Ref. 30)	$3.8\cdot 10^{-3}$
311.7		$3.60\cdot 10^{-3}$ (T; Ref. 61)	$4.2\cdot 10^{-3}$
312.8		$5.60\cdot 10^{-3}$ (T; Ref. 58)	$4.4\cdot 10^{-3}$
313.2	100 (Ref. 15)	$4.16\cdot 10^{-3}$ (T; Ref. 15), $3.82\cdot 10^{-3}$ (T; Ref. 19), $3.74\cdot 10^{-3}$ (T; Ref. 47), $5.60\cdot 10^{-3}$ (T; Ref. 58)	$4.4\cdot 10^{-3}$
321.2		$4.90\cdot 10^{-3}$ (T; Ref. 61)	$5.6\cdot 10^{-3}$
323.2	100 (Ref. 15)	$5.30\cdot 10^{-3}$ (T; Ref. 15), $4.92\cdot 10^{-3}$ (T; Ref. 19), $4.85\cdot 10^{-3}$ (T; Ref. 47), $7.12\cdot 10^{-3}$ (T; Ref. 58)	$5.9\cdot 10^{-3}$
333.2	150 (Ref. 15)	$7.11\cdot 10^{-3}$ (T; Ref. 15)	$7.8\cdot 10^{-3}$
333.3		$7.88\cdot 10^{-3}$ (T; Ref. 58)	$7.8\cdot 10^{-3}$
333.7		$7.80\cdot 10^{-3}$ (T; Ref. 61)	$7.9\cdot 10^{-3}$
341.2		$1.02\cdot 10^{-2}$ (T; Ref. 61)	$9.6\cdot 10^{-3}$
343.2	250 (Ref. 15)	$9.46\cdot 10^{-3}$ (T; Ref. 15)	$1.0\cdot 10^{-2}$
343.6		$1.045\cdot 10^{-2}$ (T; Ref. 58)	$1.0\cdot 10^{-2}$
349.2		$1.29\cdot 10^{-2}$ (T; Ref. 61)	$1.2\cdot 10^{-2}$
353.2	250 (Ref. 15)	$1.28\cdot 10^{-2}$ (T; Ref. 15)	$1.3\cdot 10^{-2}$
354.2		$1.251\cdot 10^{-2}$ (T; Ref. 58)	$1.3\cdot 10^{-2}$
357.2		$1.58\cdot 10^{-2}$ (T; Ref. 61)	$1.4\cdot 10^{-2}$
363.2	350 (Ref. 15)	$1.62\cdot 10^{-2}$ (T; Ref. 15)	$1.7\cdot 10^{-2}$
363.4		$1.421\cdot 10^{-2}$ (T; Ref. 58)	$1.7\cdot 10^{-2}$
366.2		$2.08\cdot 10^{-2}$ (T; Ref. 61)	$1.8\cdot 10^{-2}$
372.6	153 (Ref. 1)	$1.923\cdot 10^{-2}$ (T; Ref. 1)	$2.1\cdot 10^{-2}$
373.2	350 (Ref. 15)	$2.26\cdot 10^{-2}$ (T; Ref. 15)	$2.1\cdot 10^{-2}$
398.0	384 (Ref. 1)	$3.411\cdot 10^{-2}$ (T; Ref. 1)	$3.7\cdot 10^{-2}$
422.6	753 (Ref. 1)	$5.789\cdot 10^{-2}$ (T; Ref. 1)	$6.1\cdot 10^{-2}$
422.8	6800 (Ref. 11)	$5.80\cdot 10^{-2}$ (T; Ref. 11)	$6.1\cdot 10^{-2}$
429.2	6800 (Ref. 11)	$7.30\cdot 10^{-2}$ (T; Ref. 11)	$7.0\cdot 10^{-2}$
448.4	1425(Ref. 1)	$9.826\cdot 10^{-2}$ (T; Ref. 1)	$1.0\cdot 10^{-1}$
448.5	1404 (Ref. 1)	$9.525\cdot 10^{-2}$ (T; Ref. 1)	$1.0\cdot 10^{-1}$
451.1	6800 (Ref. 11)	$9.80\cdot 10^{-2}$ (T; Ref. 11)	$1.1\cdot 10^{-1}$
453.3	6800 (Ref. 11)	$1.05\cdot 10^{-1}$ (T; Ref. 11)	$1.1\cdot 10^{-1}$
467.8	6800 (Ref. 11)	$1.34\cdot 10^{-1}$ (T; Ref. 11)	$1.4\cdot 10^{-1}$
470.9	6800 (Ref. 11)	$1.45\cdot 10^{-1}$ (T; Ref. 11)	$1.5\cdot 10^{-1}$
473.2	2500 (Ref. 14)	$2.32\cdot 10^{-1}$ (D; Ref. 14)	$1.6\cdot 10^{-1}$
473.6	2363 (Ref. 1)	$1.592\cdot 10^{-1}$ (T; Ref. 1)	$1.6\cdot 10^{-1}$
479.8	6800 (Ref. 11)	$1.65\cdot 10^{-1}$ (T; Ref. 11)	$1.8\cdot 10^{-1}$
485.1	6800 (Ref. 11)	$1.82\cdot 10^{-1}$ (T; Ref. 11)	$2.0\cdot 10^{-1}$
488.4	6800 (Ref. 11)	$1.91\cdot 10^{-1}$ (T; Ref. 11)	$2.1\cdot 10^{-1}$
494.7	6800 (Ref. 11)	$2.14\cdot 10^{-1}$ (T; Ref. 11)	$2.3\cdot 10^{-1}$
502.5	6800 (Ref. 11)	$2.53\cdot 10^{-1}$ (T; Ref. 11)	$2.6\cdot 10^{-1}$
504.2	6800 (Ref. 11)	$2.41\cdot 10^{-1}$ (T; Ref. 11)	$2.7\cdot 10^{-1}$
513.5	6800 (Ref. 11)	$2.88\cdot 10^{-1}$ (T; Ref. 11)	$3.2\cdot 10^{-1}$
521.6	6800 (Ref. 11)	$3.29\cdot 10^{-1}$ (T; Ref. 11)	$3.6\cdot 10^{-1}$
523.2	5800 (Ref. 14)	$3.84\cdot 10^{-1}$ (T; Ref. 14)	$3.7\cdot 10^{-1}$
524.3	6800 (Ref. 11)	$3.47\cdot 10^{-1}$ (T; Ref. 11)	$3.8\cdot 10^{-1}$
548.2	8600 (Ref. 14)	$5.69\cdot 10^{-1}$ (T; Ref. 14)	$5.5\cdot 10^{-1}$

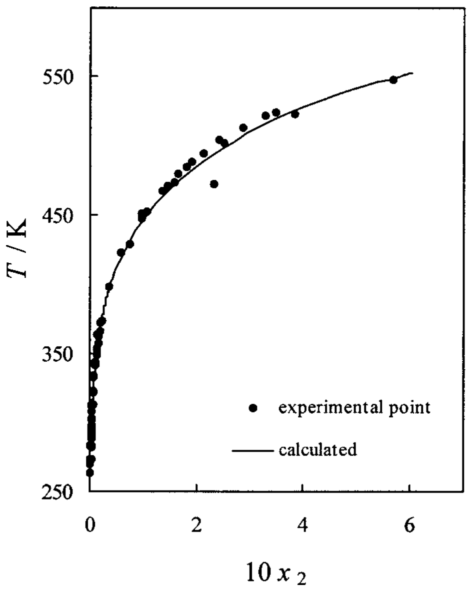

FIG. 3. All the solubility data for water (2) in toluene (1).

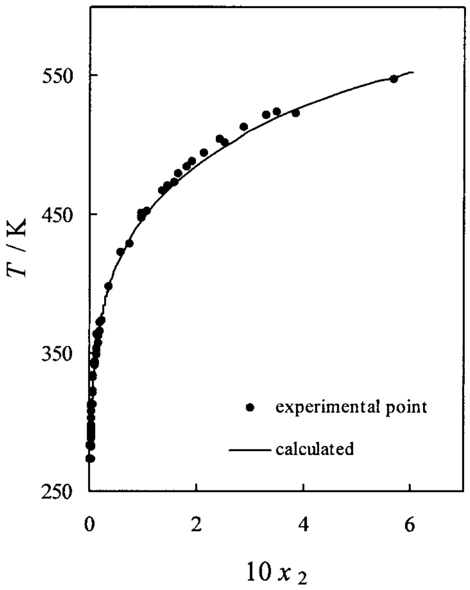

FIG. 4. Recommended and tentative solubility data for water (2) in toluene (1).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	F. E. Anderson and J. M. Prausnitz, Fluid Phase Equilib. **32**, 63 (1986).
Variables:	**Prepared By:**
Temperature: 99.4 °C–200.4 °C Pressure: 1.53–23.63 bar	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

t/°C	P/bar	$g(1)$/100 g sln (compilers)	$10^3 \cdot x_1$
99.4	1.53	0.146	0.286±0.017
124.8	3.84	0.236	0.463±0.015
149.4	7.53	0.405	0.794±0.030
175.2	14.25	0.661	1.30±0.023
175.3	14.04	0.626	1.23±0.027
200.4	23.63	1.311	2.59±0.110

Solubility of water in toluene

t/°C	P/bar	$g(2)$/100 g sln (compilers)	X_2
99.4	1.53	0.382	0.01923±0.00035
124.8	3.84	0.686	0.03411±0.00044
149.4	7.53	1.187	0.05789±0.00080
175.2	14.25	2.086	0.09826±0.00075
175.3	14.04	2.017	0.09525±0.00170
200.4	23.63	3.570	0.15920±0.00160

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The equilibrium cell, about 140 mL, was filled with a mixture of (1) and (2), temperature controllers were set at the desired temperature, liquids were degassed, agitated and allowed to reach equilibrium for 2 h. Details of the apparatus and sampling procedures were described in the paper. Temperatures were measured by a resistance temperature detector. All analyses were made using a gas chromatograph equipped with a thermal-conductivity detector. Mean values of 5–10 replicated measurement were reported.

Source and Purity of Materials:

(1) Source not specified; spectral grade reagent; used as received.
(2) Purified and deionized by adsorption on activated carbon.

Estimated Error:

Temperature: ±0.5°C.
Solubility: standard deviation as above.
Pressure: ±0.1 bar.

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.053 $g(1)/100$ g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $1.04 \cdot 10^{-4}$.

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 a Beckman spectrophotometer.

Source and Purity of Materials:

(1) Eastman Kodak Co. best grade; washed successively with concentrated sulfuric acid, water, and dilute sodium hydroxide; dried, and distilled; b.p. 110.4 °C.
(2) Not specified.

Estimated Error:
Not specified.

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	S. Banerjee, Environ. Sci. Technol. **18**, 587 (1984).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

$t/°C$	mg (1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
25.0	524	$5.25 \cdot 10^{-2}$	$1.027 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A tube containing 50 mg–2 g of component (1) and 5–10 mL of water was shaken for at least 48 h and then allowed to separate for 24 h. Following equilibration, the water-rich phase in the tube was sampled at least in duplicate, the solution was diluted with an equal volume of acetonitrile to prevent any deposition of material and then analyzed by high-pressure liquid chromatography. A Waters Associates M6000A pump fitted with either a Lichrosorb RP-2 or an Altex Ultrasphere ODS column and a LDC Spectromonitor III detector was used.

Source and Purity of Materials:

(1) Not specified.
(2) Distilled water.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: about 5% (standard error of replicate determinations).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
Variables:	**Prepared By:**
One temperature: 25 °C	G. T. Hefter

Experimental Data

The solubility of toluene in water was reported to be $1.68 \cdot 10^{-2}$ mol/L sln.

Assuming a solution density of 1.00 kg/L the corresponding mass percent and mole fraction, x_1, solubilities, calculated by the compiler, are 0.155 $g(1)$/100 g sln and $3.04 \cdot 10^{-4}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of radio-labeled toulene was added to a tube contained distilled water, and the tube was sealed and allowed to equilibrate at 25±0.2 °C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10 000 rpm for 60 min in a head preequilibrated 25±0.3 °C, following which aliquots of the solution were removed for analysis by liquid scintillation counting. The entire procedure was carried out at least twice, and each analysis was also conducted in duplicate.

Source and Purity of Materials:

(1) ^{14}C-labeled toluene: New England Nuclear, used without further purification.
(2) Distilled.

Estimated Error:

Temperature: ±0.2 °C.
Solubility: ±2.3% rel. (representing 1 standard deviatiion).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	V. G. Benkovski, M. H. Nauruzov, and T. M. Bogoslovskaya, Tr. Inst. Khim. Nefti Prir. Solei, Akad. Nauk Kaz. SSR **2**, 25 (1970).
Variables:	**Prepared By:**
One temperature: 303 K	A. Maczynski

Experimental Data

The solubility of water in toluene at 303 K was reported to be 0.0273 $g(2)$/100 g sln.

The corresponding mole fraction, x_1, value calculated by compiler is 0.0739.

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) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	A. Ben-Naim and J. Wilf, J. Phys. Chem. **70**, 771 (1979).
Variables:	**Prepared By:**
Temperature: 10.0 °C and 20.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

$t/°C$	$10^3 \cdot mol(1)/L$ sln	$10^2 \cdot g(1)/100$ g sln (compilers)	$10^4 \cdot x_1$ (compilers)
10.0	6.21	5.72	1.119
20.0	6.37	5.87	1.149

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Fluka, puriss grade, ⩾99.5%; used as received.
(2) Triple distilled.

Estimated Error:

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

References:

[1] A. Ben-Naim, J. Wilf, and M. Yaacobi, J. Phys. Chem. **77**, 95 (1973).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	A. Ben-Naim and J. Wilf, J. Phys. Chem. **84**, 583 (1980).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of water in toluene

$t/°C$	mol (1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
25.0	$6.69 \cdot 10^{-3}$	$6.18 \cdot 10^{-2}$	$1.209 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Water (2) with an excess of toluene (!) was stirred for about 48 h in a thermostat and then the two phases were allowed to separate for about 24 h. Samples were analyzed spectroscopically in the UV region by a Perkin-Elmer model 450 spectrophotometer.
Confirming results were obtained through contact between water and the vapor of the solute; the method was described in Ben-Naim *et al.*[1]

Source and Purity of Materials:

(1) Fluka, puriss grade, 99.9%; used as received.
(2) Triple distilled.

Estimated Error:

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

References:

[1] A. Ben-Naim, J. Wilf, and M. Yaacobi, J. Phys. Chem. **77**, 95 (1973).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8 ; [108-88-3] (2) Water; H_2O; [7732-18-5]	R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
Variables:	**Prepared By:**
Temperature: 0.4 °C–45.3 °C	G. T. Hefter

Experimental Data

Solubility of toluene in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln[a] (compiler)
0.4	1.29	0.0658
3.6	1.26	0.0646
10.0	1.23	0.0628
11.2	1.22	0.0624
14.9	1.22	0.0623
15.9	1.21	0.0621
25.0	1.23[b]	0.0627[b]
25.6	1.22	0.0625
30.0	1.25	0.0640
30.2	1.25	0.0642
35.2	1.28	0.0657
42.8	1.37	0.0701
45.3	1.40	0.0717

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

[b] Given in the original paper as 0.627 $g(1)$/L sln.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Phillips Petroleum Co., 99+%, used as received.
(2) Air-free conductivity water, no further details given.

Estimated Error:

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

Components:	**Original Measurements:**
(1) Toluene; C_7H_8 ; [108-88-3] (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: 25.0 °C (298.2 K)	G. T. Hefter

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.04 mL (1)/100 mL (2).

The solubility of (1) in 40.0% (w/w?) aqueous sodium xylene sulfonate solution was also reported to be 1.20 mL (1)/100 mL sulfonate sln.

Auxiliary Information

Method/Apparatus/Procedure:

A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.02 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute, measured directly in the tube, from the total added.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:

(1) Toluene; C_7H_8 ; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. S. Bradley, M. J. Dew, and D. C. Munro, High Temperature:-High Pressures **5**, 169 (1973).

Variables:

Temperature: 25 °C–55 °C
Pressure: 1 and 1200 bar

Prepared By:

G. T. Hefter

Experimental Data

Solubility of toluene in water

$t/°C$	$10^4 \cdot x_1$[a] (compiler)	$g(1)/100$ g sln[a] (compiler)	mol (1)/L sln	P/bar[b]
25	1.07	0.0547	0.00595	1
45	1.41	0.0722	0.00785	1
55	1.68	0.086	0.0094	1
45	2.17	0.111	0.0121	1000
55	2.37	0.121	0.0131	1000

[a] Assuming a solution density of 1.00 kg/L at all temperatures.

[b] 1 bar = 0.1 MPa exactly.

Data at other pressures are presented in graphical form. Data are also presented for the solubility of (1) in aqueous solutions of $AgNO_3$ and KNO_3 at various temperatures and pressures.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) at room temperature and pressure was determined in a stoppered 1 mm silica cuvette placed in a Unicam SP500 spectrophotometer and stirred magnetically. Measurements were made until a constant concentration was reached. The value was checked against a 2 L sample of saturated solution which had been equilibrated for some months.

Solubilities at higher temperature and pressure were similarly determined in a special cell fitted into the spectrophotometer. Many details of the apparatus are given in the paper.

Source and Purity of Materials:

(1) Not specified.
(2) Distilled, air-free.

Estimated Error:

Not specified.

Components:

(1) Toluene; C_7H_8 ; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. S. Brown, J. P. Hallett, D. Bush, and C. A. Eckert, J. Chem. Eng. Data **45**, 846 (2000).

Variables:

Temperature: 340.6 K–524.3 K
Pressure: 6.80 MPa

Prepared By:

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

Experimental Data

Solubility of toluene in water

T/K	P/MPa	$g(1)/100$ g sln (compiler)	$10^3 \cdot x_1$
340.6	6.80	0.093	0.183±0.005
384.1	6.80	0.184	0.360±0.008
403.2	6.80	0.269	0.527±0.010
417.2	6.80	0.353	0.693±0.011
445.0	6.80	0.600	1.18±0.02
485.2	6.80	1.36	2.68±0.05
518.0	6.80	2.74	5.47±0.11

Solubility of water in toluene

T/K	P/MPa	$g(2)/100$ g sln (compiler)	x_2
524.3	6.80	9.41	0.347±0.03
521.6	6.80	8.75	0.329±0.03
513.5	6.80	7.33	0.288±0.03
502.5	6.80	6.21	0.253±0.03
504.2	6.80	5.85	0.241±0.03
494.7	6.80	5.05	0.214±0.03
488.4	6.80	4.41	0.191±0.02
485.1	6.80	4.17	0.182±0.03
479.8	6.80	3.72	0.165±0.02
470.9	6.80	3.21	0.145±0.02
467.8	6.80	2.94	0.134±0.02
453.3	6.80	2.24	0.105±0.02
451.1	6.80	2.08	0.098±0.02
429.2	6.80	1.52	0.073±0.03
422.8	6.80	1.19	0.058±0.02

Auxiliary Information

Method/Apparatus/Procedure:

The cloud point method was used. Solubilities were measured in a variable-volume windowed vessel (20 mL maximum volume), described in Ref. 1, and placed in a thermostated air bath (modified Varian 3400 gas chromatograph). Apparatus and procedure were described in detail in the paper. Temperature was measured with a hand-held readout (HH22 Omega) and thermocouple (Omega type K). The pressure was measured with a Druck DPI 260 gauge with PDCR 910 transducer.

Source and Purity of Materials:

(1) Aldrich Chemicals Co.; HPLC grade purity 99.8 mass %; used as received.
(2) Aldrich Chemicals Co.; HPLC grade.

Estimated Error:

Temperature: ±0.2 K (precision of measurements), ±1 K (reproducibility).
Pressure: ±0.001 MPa.
Solubility: as above.

References:

[1] C. F. Kirby and M. A. McHugh, Chem. Rev. **99**, 565 (1999).

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A **78**, 453 (1974).

Variables:

Temperatures: 4.5 °C–20.1 °C (277.7 K–293.3 K)

Prepared By:

G. T. Hefter

Experimental Data

Solubility of toluene in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln[a]
4.5	1.20	0.0612±0.0010
6.3	1.18	0.0601±0.0011
7.1	1.15	0.0586±0.0018
9.0	1.15	0.0587±0.0011
11.8	1.12	0.0573±0.0014
12.1	1.13	0.0575±0.0012
15.1	1.11	0.0569±0.0013
17.9	1.13	0.0577±0.0013
20.1	1.11	0.0566±0.0011

[a] Errors given as standard deviation.

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography.

The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. Basically, the hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

Source and Purity of Materials:

(1) 99.99 mole % purity; source and methods of purification not specified.
(2) Distilled.

Estimated Error:

Temperature: ±0.01 °C.
Solubility: see table above.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. D. Caddock and P. L. Davies, J. Inst. Pet. **46**, 391 (1960).

Variables:

One temperature: 20 °C

Prepared By:

A. Maczynski

Experimental Data

The solubility of water in toluene at 20 °C was reported to be 46 mg (2)/100 g (1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.046 $g(2)$/100 g sln and 0.0023.

Auxiliary Information

Method/Apparatus/Procedure:

A sample of (1) was equilibrated at 20 °C with an air stream containing a known amount of water vapor tagged with HTO. At equilibrium a sample of (1) was taken and its (2) content determined by liquid scintillation counting.

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±0.01 °C.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Fluka, puriss grade, purity ⩾99.5%; used as received.
(2) Triply distilled.

Estimated Error:

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

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

K. Chandler, B. Eason, C. L. Liotta, and C. A. Eckert, Ind. Eng. Chem. Res. **37**, 3515 (1998).

Variables:

Temperature: 200 °C–275 °C
Pressure: 25 bar–172 bar

Prepared By:

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

Experimental Data

Solubility of toluene in water

$t/°C$	P/bar	$g(1)/100$ g sln (compilers)	$10^2 \cdot x_1$
200	25	1.21	0.238±0.017
250	58	3.49	0.703±0.095
250	172[a]	3.55	0.714±0.029
275	86	6.27	1.29±0.06
275	172[a]	6.27	1.29±0.04

Solubility of water in toluene

$t/°C$	P/bar	$g(2)/100$ g sln (compilers)	x_2
200	25	5.58	0.232±0.031
250	58	10.86	0.384±0.032
250	172[a]	8.97	0.335±0.013
275	86	20.52	0.569±0.015
275	172[a]	13.94	0.453±0.015

[a] Pressure above the three-phase pressure.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A commercially available 300 mL stainless steel sample cylinder (Whitey Co.) as an equilibrium cell, a temperature controller (Omega Engineering, Inc.) and a digital pressure transducer (Heise, 901B) were used. Details of the apparatus and sampling procedures were described in the paper. Samples were analyzed with a glc (Varian Model 3400) equipped with a thermal conductivity detector for the water-rich phase and equipped with FID detector for the hydrocarbon-rich phase. 5–10 replicated measurements at each point were made.

Source and Purity of Materials:

(1) Aldrich Chemicals Co.; HPLC grade reagent; purity >99.8%; used as received.
(2) Aldrich Chemicals Co.; HPLC grade water.

Estimated Error:

Temperature: ±1 °C.
Pressure: ±0.3 bar.
Solubility: standard deviation as above.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 475 (1994).

Variables:

Temperature: 303.15 K–373.15 K
Pressure: 1.0 bar–3.5 bar

Prepared By:

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

Experimental Data

Solubility of toluene in water

T/K	P/bar	$g(1)/100$ g sln (compilers)	$10^4 \cdot x_1$
303.15	1.0	0.0598	1.17±0.026
313.15	1.0	0.0608	1.19±0.036
323.15	1.0	0.0649	1.27±0.014
333.15	1.5	0.0736	1.44±0.036
343.15	2.5	0.0874	1.71±0.055
353.15	2.5	0.1012	1.98±0.056
363.15	3.5	0.1185	2.32±0.024
373.15	3.5	0.1369	2.68±0.060

Solubility of water in toluene

T/K	P/bar	$g(2)/100$ g sln (compilers)	$10^2 \cdot x_2$
303.15	1.0	0.0570	0.291±0.019
313.15	1.0	0.0816	0.416±0.006
323.15	1.0	0.1041	0.530±0.039
333.15	1.5	0.1398	0.711±0.020
343.15	2.5	0.1864	0.946±0.026
353.15	2.5	0.2529	1.28±0.06
363.15	3.5	0.3209	1.62±0.05
373.15	3.5	0.4501	2.26±0.10

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The 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 dehydrated ethanol or 2,2,4-trimethylpentane as a solvent. Details of the standard preparation, calibration, and sampling procedures were described in the paper. A Hewlett-Packard 5880A gas chromatograph equipped with Poropac or Glas Chrom 254 columns and a thermal conductivity detector were used for analysis. Reported solubilities are the average of 6–13 replicate determinations.

Source and Purity of Materials:

(1) Aldrich Chemical Co.; purity >99.9%; used as received.
(2) Distilled and deionized water.

Estimated Error:

Temperature: ±0.2 K (compilers).
Solubility: standard deviation as above.

References:

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

Components:
(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. Chey and G. V. Calder, J. Chem. Eng. Data **17**, 199 (1972).

Variables:
One temperature; 21 °C

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

Experimental Data

Solubility of toluene in water

t/°C	$g(1)$/100 g sln	x_1 (compilers)
21	0.0479±0.0086	$9.36\cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A mixture containing about 50 mL of (2) and about 1 mL of (1) was allowed to stand for 10–20 h with occasional stirring in a thermostatted separatory funnel. Procedures for sampling were described in the paper. A sample was dissolved in isopropyl ether and analyzed with a Carle gas chromatograph Model 8004. The mean of three experiments was reported.

Source and Purity of Materials:

(1) Source not specified; A.R. reagent; used as received.
(2) Distilled water.

Estimated Error:

Temperature: ±1 °C.
Solubility: as above.

Components:
(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).

Variables:
Temperature: 280 °C–310 °C
Pressure: 150 atm–600 atm

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of toluene in water

t/°C	x_1 (compiler)	$g(1)$/100 g sln	P/atm	P/MPa (compiler)
280	0.0141	6.8	150	15.2
280	0.0141	6.8	250	25.3
280	0.0136	6.6	410	41.5
280	0.0119	5.8	600	60.8
300	0.0313	14.2	170	17.2
300	0.0311	14.1	250	25.3
300	0.0308	14.0	300	30.4
305	0.0411	18.0	160	16.2
305	0.0438	19.0	180	18.2
305	0.0452	19.5	200	20.3
305	0.0438	19.0	250	25.3
305	0.0411	18.0	285	28.9
310	0.0411	18.0	145	14.7
310	0.0455	19.6	150	15.2
310	0.0514	21.7	155	15.7
310	0.0578	23.9	165	16.7
310	0.0590	26.7	170	17.2
310	0.0759	29.6	175	17.7
310	0.0882	33.1	180	18.2
310	0.1002	36.3	180	18.2
310	0.1663	50.5	270	27.3
310	0.1560	48.6	265	26.9
310	0.1452	46.5	260	26.3
310	0.1346	44.3	260	26.3
310	0.1236	41.9	260	26.3
310	0.1119	39.2	260	26.3
310	0.1002	36.3	260	26.3
310	0.0882	33.1	260	26.3
310	0.0759	29.6	275	27.9
310	0.0665	26.7	295	29.9
310	0.0575	23.8	325	32.9
310	0.0452	19.5	405	41.0
310	0.0411	11.0	455	46.1

Auxiliary Information

Method/Apparatus/Procedure:

Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected until either a cloud or a small droplet of a second phase appeared at the top of the cell. Then mercury was injected to change pressure, more (1) was injected and the measurement was repeated.

Source and Purity of Materials:

(1) Phillips reagent grade; better than 99.8%; used as received.
(2) Distilled and degased.

Estimated Error:

Temperature: ±0.02 °C.
Pressure: ±2 atm.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(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 toluene in water

T/K	$10^3 \cdot$ mol(1)/L sln	$10^2 \cdot g(1)$/100 g sln (compilers)	$10^4 \cdot x_1$
273.65	6.11	5.62	1.10
278.15	5.99	5.52	1.08
288.15	5.88	5.42	1.06
298.15	6.03	5.57	1.09
308.25	6.40	5.93	1.16
318.15	6.86	6.39	1.25
328.15	7.64	7.16	1.40

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) Lachema (Czech Republic); p.a. reagent; fractionally distilled, dried, and stored with 4 A molecular sieves.
(2) Distilled and treated by a Milli-Q water purification system.

Estimated Error:

Temperature: ±0.01 K.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(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 toluene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
0	1.382	0.02704
10	1.61	0.0316
20	2.35	0.0460
30	3.14	0.0615
40	3.82	0.0750
50	4.92	0.0965

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) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. Führer, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).

Variables:

One temperature: 16 °C

Prepared By:

A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of toluene in water at 16 °C was reported to be 0.047 $g(1)/100$ g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $9.2 \cdot 10^{-5}$.

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 of (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) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. K. Glasoe and S. D. Schultz, J. Chem. Eng. Data **17**, 66 (1972).

Variables:

Temperature: 15 °C–30 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in toluene

$t/°C$	$10^3 \cdot x_2$ (compiler)	$g(2)/100$ g sln (compiler)	mol (2)/L sln
15	2.11	0.0413	0.0200±0.0006
25	2.78	0.0545	0.0261±0.0004
30	3.14	0.0615	0.0293±0.0004

The compilers calculations assume a solution density of 0.862 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

Dried (1) was saturated with (2) by allowing it to stand in contact with (2) in a closed system, protected from atmospheric moisture.

This two-phase system was kept in a pyrex storage bottle which was immersed in a constant temperature water bath.

The concentration of (2) in (1) was determined by the Karl Fischer method.

Source and Purity of Materials:

(1) Source not specified; reagent grade; purified by distillation and dried over molecular sieve.
(2) Distilled in a pyrex system.

Estimated Error:

Solubility: as indicated above (type of error not specified).

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. D. Gregory, S. D. Christian, and H. E. Affsprung, J. Phys. Chem. **71**, 2283 (1967).

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in toluene at 25 °C was reported to be 0.0268 mol (2)/L sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0560 $g(2)/100$ g sln and $2.86 \cdot 10^{-3}$. The assumption that 1 L sln=863 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

A solution of (2) in (1) was obtained using solute isopiestic equilibrator described in Christian *et al.*[1] Water concentration was determined with a Beckman KF-3 aquameter by the Karl Fischer analysis.

Source and Purity of Materials:

(1) Source not specified; reagent grade; fractionally distilled through a 30-plate Oldershaw column.
(2) Not specified.

Estimated Error:

Temperature: ±0.05 °C.

References:

[1] S. P. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, J. Chem. Educ. **40**, 419 (1963).

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

Variables:

One temperature: 30 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Data

The solubility of toluene in water at 30 °C was reported to be 0.57 $g(1)/\text{kg}(2)$ and 0.0062 mol (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.057 $g(1)/100$ g sln and $1.12 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared by shaking in a thermostat and were analyzed by means of an interferometer. The instrument used was a combination liquid and gas interferometer made by Zeiss.

Source and Purity of Materials:

(1) Baker's CP analyzed grade; distilled; b.p. 110.74 ±0.02 °C.
(2) Distilled.

Estimated Error:

Solubility: 2.0% (from values of duplicate determinations).

Components:

(1) Toluene; C_7H_8; [108-88-3]
(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); Radiokhimiya, **5**, 507 (1963).

Variables:

Temperature: 90 °C–224 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Data

Solubility of toluene in water

t/°C	$10^3 \cdot x_1$ (compiler)	$g(1)$/100 g sln
90	0.83	0.42
114	1.619	0.823
147	3.248	1.640
169	4.737	2.387
183	5.579	2.790
207	8.314	4.113
224	10.336	5.072

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}1.4970.
(2) Doubly distilled.

Estimated Error:

Not specified.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. Haruki, Y. Iwai, S. Nagao, and Y. Arai, J. Chem. Eng. Data **46**, 950 (2001).

Variables:

Temperature: 573.2 K and 583.2 K
Pressure: 10.5 MPa– 28.1 MPa

Prepared By:

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

Experimental Data

Mutual solubility of toluene in water

T/K	P/MPa	$g(1)$/100 g sln (compilers)	x_1
573.2	13.6	0.116	0.025 ± 0.0013
	15.3	0.116	0.025 ± 0.0011
583.2	18.3	0.201	0.047 ± 0.0012
	20.4	0.205	0.048 ± 0.0009
	22.2	0.205	0.048 ± 0.0019
	25.2	0.194	0.045 ± 0.0008
	28.1	0.190	0.044 ± 0.0011

Mutual solubility of water in toluene

T/K	P/MPa	$g(2)$/100 g sln (compilers)	x_2
573.2	10.5	56.9	0.871 ± 0.0190
	11.2	49.9	0.836 ± 0.0060
	12.3	35.8	0.740 ± 0.0130
	13.6	31.5	0.702 ± 0.0096
	15.3	30.7	0.694 ± 0.0067
583.2	11.4	69.2	0.920 ± 0.0083
	12.6	51.2	0.843 ± 0.0063
	13.6	41.9	0.787 ± 0.0119
	15.2	41.2	0.782 ± 0.0081
	18.3	42.4	0.790 ± 0.0083
	20.4	42.5	0.791 ± 0.0061
	22.2	41.2	0.782 ± 0.0080
	25.2	38.1	0.759 ± 0.0055
	28.1	36.4	0.745 ± 0.0076

Auxiliary Information

Method/Apparatus/Procedure:

A flow-type apparatus to measure the phase equilibria at high temperatures and pressures was used, details were described in Haruki *et al.*[1] Pressure was controlled by back-pressure regulators. The phase behavior was observed with a video camera attached to a telescope. Samples of each phase were collected in bottles containing ethanol to obtain homogenous solutions. The compositions of samples were analyzed by a gas chromatograph with a thermal conductivity detector. Solubilities reported are the arithmetic average of 6–17 experimental points.

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±1 K.
Pressure: ±0.1 MPa.

References:

[1] M. Haruki, Y. Iwai, S. Nagao, Y. Yahiro, and Y. Arai, J. Chem. Eng. Res. **39**, 4516 (2000).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).
Variables: One temperature: 25 °C	**Prepared By:** A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in toluene was reported to be 0.026 mol (2)/L sln.

The corresponding mass percent and mol fraction, x_2, calculated by the compilers are 0.054 $g(2)$/100 g sln and $2.8 \cdot 10^{-3}$. The assumption that 1 L sln = 862 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

The water determination was carried out according to Johansson's modification of the Karl Fischer titration in Hardy *et al.*[1] and Johansson.[2]

Source and Purity of Materials:

(1) Kebo; purity 99.0%; used as received.
(2) Not specified.

Estimated Error:

Temperature: ±0.3 °C.
Solubility: ±0.001 mol(2)/L sln (type of error not specified).

References:

[1] C. J. Hardy, B. F. Greenfield, and D. Scargill, J. Chem. Soc. **90** (1961).

[2] A. Johansson, Sv. Papperstidn. **11B**, 124 (1947).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	A. Jäger, Brennst.-Chem. **4**, 259 (1923).
Variables: Temperature: 100 °C–300 °C	**Prepared By:** A. Maczynski

Experimental Data

Solubility of toluene in water

t/°C	mL (1)/100 mL (2)
150	0.2
200	0.7
250	2.8
300	13.0

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined in sealed glass tubes.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	J. R. Johnson, S. D. Christian, and H. E. Affsprung, J. Chem. Soc. A **77** (1966).
Variables: One temperature: 25 °C	**Prepared By:** A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in toluene at 25 °C was reported to be 0.0274 mol (2)/L sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0572 $g(2)/100$ g sln and $2.92 \cdot 10^{-3}$. The assumption that 1 L sln=862 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus described in Christian *et al.*[1] was used without modification. Samples were equilibrated in a constant-temperature water bath maintained at 25±0.1 °C. Water solubilities were determined by using a Beckman Model KF-3 Aquameter.

Source and Purity of Materials:

(1) Source not specified; certified or reagent grade; distilled through a 30-plate Oldershaw column.
(2) Not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±0.0005 mol(2)/L sln (type of error not specified).

References:

[1] S. P. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, J. Chem. Educ. **40**, 419 (1963).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	J. R. Jones and C. B. Monk, J. Chem. Soc. 2633 (1963).
Variables: Temperature: 25 °C–35 °C	**Prepared By:** A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

Solubility of water in toluene

$t/°C$	$10^4 \cdot mL(2)/mL(1)$
25	4.0
30	4.8
35	5.9

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) "Analar" grade; repurified by conventional methods, Vogel.[1]
(2) Not specified.

Estimated Error:

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

References:

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

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **33**, 87 (1988).
Variables: One temperature: 25.00 °C	**Prepared By:** A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

t/°C	mol (1)/L sln	$g(1)$100 g sln (compilers)	x_1
25.00	$(6.29\pm0.03)\cdot10^{-3}$	$5.78\cdot10^{-2}$	$(1.13\pm0.01)\cdot10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were determined by headspace chromatographic analysis[1] using a multiple injection interrupted flow technique. Samples were prepared in septum bottles of 160 mL volume which were thermostated and shaken for 72 h prior to analysis. For analysis each bottle was transferred to a tempering beaker and pressurized to 15.00 psig with chromatographic grade nitrogen. Bottles were attached to the headspace sampling port of a gas chromatograph with a flame ionization detector. Solubility was calculated on the bases of Henry's law.

Source and Purity of Materials:

(1) Baker Instruments; analyzed grade; purity 99.83% by glc.
(2) Deionized water.

Estimated Error:

Temperature: ±0.01 °C.
Solubility: as above (standard deviation of the mean).

References:

[1] D. F. Keeley and J. R. Meriwether, Rev. Sci. Instrum. **75**, 1434 (1986).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables: Temperature: 25 °C	**Prepared By:** M. C. Haulait-Pirson

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.500 $g(1)$/L sln and 0.00543 mol (1)/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler assuming a solution density of 1.00 g/mL are 0.05 $g(1)$/100 g sln and $9.80\cdot10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Zh. Prikl. Khim. (Leningrad) **51**, 957 (1978).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.65 $g(1)/\mathrm{L}$ sln

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.065 $g(1)/100$ g sln and $1.27 \cdot 10^{-4}$. The compiler's calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

About 200–500 mL (2) was placed in a ground-joint glass cylinder and 20–50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).

Source and Purity of Materials:

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

Estimated Error:

Solubility: ±0.01 g(1)/L sln (standard deviation from 6 determinations).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 1977.04.05.
Variables:	**Prepared By:**
One temperature: 20 °C	A. Maczynski

Experimental Data

The solubility of toluene in water at 20 °C was reported to be 0.57 $g(1)/\mathrm{L}(2)$.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.057 $g(1)/100$ g sln and $1.11 \cdot 10^{-4}$. The compiler's calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

About 100–500 mL (2) was placed in a glass cylinder and 10–50 mg of an insoluble indicator was added and (1) was microburretted until the indicator floated to form a colored thin layer on the cylinder wall 2–3 cm above the liquid layer. After each drop or (1), the mixture was vigorously mixed for 0.5–1.5 min.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified

Estimated Error:

Not specified.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(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 toluene in water at 25 °C was reported to be 0.220 mg (1)/mL sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.022 $g(1)$/100 g sln and $4.3\cdot 10^{-5}$. The compiler's calculations assume a solution density of 1.00 g/mL.

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 90–140 °C.

Source and Purity of Materials:

(1) Described in Ref. 1.
(2) Distilled.

Estimated Error:

Temperature: ±1 °C.

References:

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

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. M. Lo, C. L. Tseng, and J. Y. Yang, Anal. Chem. **58**, 1596 (1986).

Variables:

One temperature: 25 °C

Prepared By:

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

Experimental Data

Solubility of toluene in water

$t/°C$	$g(1)/100$ g sln	x_1 (compilers)
25	0.052 ± 0.002	$1.02\cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:

The radiometric method was used. The radioagent $^{60}Co(PDC)_3$ was first dissolved in component (1) before pure water was added. Both of the liquids were placed in a 1000 mL separation funnel. The mixture was shaken for 5 min and allowed to separate for next 30 min. Concentration was calculated from activity measurements by a NaI(Tl) scintillation detector.

Source and Purity of Materials:

(1) E. Merck; purity not specified.
(2) Demineralized and degassed.

Estimated Error:

Solubility: as above (standard deviation of mean).

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. H. Y. Ma, H. Hung, W.-Y. Shiu, and D. Mackay, J. Chem. Eng. Data **46**, 619 (2001).

Variables:

Temperature: 5.0 °C–45.0 °C

Prepared By:

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

Experimental Data

Solubility of toluene in water

$t/°C$	$g(1)/m^3$	$10^2 \cdot g(1)/100$ g sln (compilers)	$10^4 \cdot x_1$ (compilers)
5.0	540±29	5.42	1.056
15.0	516±16	5.16	1.010
25.0	519±5.0	5.21	1.018
35.0	555±30	5.57	1.091
45.0	632±21	6.39	1.248

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Saturated solutions were prepared by adding an excess of (1) to a 125 mL or 250 mL Erlenmeyer flask containing (2). The flask was shaken and magnetically stirred for 24 h, and next allowed to settle in a constant temperature bath (Neslab Model RTE-8) for at least 48 h. A Hewlett-Packard Model 5700A GLC equipped with a flame ionization detector was used for analysis of hexane extracts. All experimental points are the mean of more than 9 determinations.

Source and Purity of Materials:

(1) Caledon Laboratories, Georgetown, Ontario; HPLC grade; used as received.
(2) Double distilled or Milli-Q ultrapure deionized water.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: as above.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.5195 $g(1)$/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.05195 $g(1)$/100 g sln and $1.015 \cdot 10^{-4}$. The compiler's calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by gas chromatography. The gas chromatograph was a Hewlett-Packard Model 5750 equipped with a hydrogen flame ionization detector. Many details are given in the paper.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; research grade; 99.9+%; used as received.
(2) Not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±0.0096 g(1)/L.

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (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 toluene in water at 25 °C was reported to be 515 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0515 $g(1)/100$ g sln and $1.01 \cdot 10^{-4}$.

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 conjunction 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: 17 mg (1)/kg (2) (standard deviation of mean).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (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 toluene in water at 25 °C was reported to be 0.0538 $g(1)/100$ g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $1.05 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:

The saturated solutions of (1) in (2) was prepared by either shaking vigorously 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: 0.0017 (standard deviation of mean).

Components:
(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 298.0 K–473.0 K
Pressure: 50 bar

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

Experimental Data

Solubility of toluene in water

T/K	P/bar	$g(1)$/100 g sln (compilers)	$10^3 \cdot x_1$
298.0	50	0.0547	0.107 ± 0.002
323.0	50	0.0639	0.125 ± 0.004
373.0	50	0.138	0.27 ± 0.01
423.0	50	0.337	0.66 ± 0.03
473.0	50	0.964	1.9 ± 0.1

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:
(1) Sigma-Aldrich, Milwaukee, WI.; purity >99%; used as received.
(2) Not stated.

Estimated Error:
Temperature: ±0.1 K.
Solubility: as above.

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

Components:
(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and F. Billett, J. Chem. Soc. 3819 (1952).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.00582 mol (1)/1000 g (2).

The corresponding mass percent and mole fraction, x_1, calculated by compilers are 0.0536 $g(1)$/100 g sln and $x_1 = 1.05 \cdot 10^{-4}$. The compiler's calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

After an excess of (1) had been shaken with about 1 L of (2) for about 1 week, a known volume of saturated solution was made slightly alkaline, and a stream of pure air passed through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in soda-asbestos. The precautions usual in organic combustions were taken.

Source and Purity of Materials:
(1) Source not specified; purest obtainable material; distilled; purity not specified.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.5% (mean of large numbers of determinations).

Components:

(1) Toluene; C_7H_8 ; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

N. Peschke and S. I. Sandler, J. Chem. Eng. Data **40**, 315 (1995).

Variables:

One temperature: 25.0 °C

Prepared By:

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

Experimental Data

Solubility of water in toluene

t/°C	$g(2)$/100 g sln (compilers)	x_2
25.0	0.045	0.0023

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The equilibrium vessel, described in the paper, was thermostatically jacketed to maintain temperature within ±0.1 °C. Mixtures of (1) and (2) were stirred for several hours before allowing a 12 h period for phase separation prior to sampling. Analysis was done using a Hewlett-Packard Model 5730 gas chromatograph with a thermal conductivity detector and a Poropak Q column.

Source and Purity of Materials:

(1) Aldrich Chemical Co; glc grade, purity 99.9 mass %; used as received.
(2) Deionized water.

Estimated Error:

Temperature: ±0.1 °C.

Components:

(1) Toluene; C_7H_8 ; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).

Variables:

Temperature: 278.16 K–318.46 K

Prepared By:

M. C. Haulait-Pirson

Experimental Data

Solubility of toluene in water

T/K	$10^3 \cdot x_1$	$g(1)$/100 g sln
278.16	0.1243	0.06357±0.0017
283.06	0.1236	0.06324±0.0016
293.06	0.1292	0.06606±0.0018
298.16	0.1232	0.06299±0.0013
308.26	0.1314	0.06721±0.0011
318.46	0.1313	0.06717±0.0020

Auxiliary Information

Method/Apparatus/Procedure:

10 mL of (2) were placed along with 4–10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 h. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 h. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.

Source and Purity of Materials:

(1) Fisher Scientific Co., Chromatoquality; 99+ mole %; used as received.
(2) Laboratory distilled water.

Estimated Error:

Solubility: standard deviation, from at least 15 measurements are given above.

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).
Variables:	**Prepared By:**
Temperature: 0 °C–25 °C	A. Maczynski and Z. Maczynska

Experimental Data

Solubility of toluene in water

$t/°C$	$10^4 \cdot x_1$ (compiler)	$g(1)/100$ g sln (compiler)	mg (1)/kg(2)
0^a	1.42	0.0724	724^c
25^b	1.12	0.0573	573^c

Solubility of water in toluene

$t/°C$	$10^3 \cdot x_2$ (compiler)	$g(2)/100$ g sln (compiler)	mg (2)/kg(1)
0^a	1.17	0.0228	228^d
25^b	2.77	0.0543	543^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 Hypovial 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) Matheson, Coleman and Bell, spectroquality grade reagent; shaken three times with distilled water.
(2) Distilled.

Estimated Error:

Temperature: (a) ±0.02 °C; (b) ±0.01 °C.
Solubility: (c) ±1.7%; (d) ±4.7%; (e) ±3.1% (mean).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (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 toluene in water at 25 °C was reported to be 554.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0554 $g(1)/100$ g sln and $1.08 \cdot 10^{-4}$.

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: ±15 mg(1)/kg(2).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	C. K. Rosenbaum and J. H. Walton, J. Am. Chem. Soc. **52**, 3568 (1930).
Variables:	**Prepared By:**
Temperature: 10 °C–50 °C	A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in toluene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	1.71	0.0335
20	2.30	0.0450
30	3.06	0.0600
40	3.74	0.0733
50	4.85	0.0953

Auxiliary Information

Method/Apparatus/Procedure:

The organic phase was first saturated by shaking with water in a flask at a high temperature and then allowing the flask to cool in a thermostat to the desired temperature, with the resulting separation of excess water. After 1 day or more the solution was allowed to react with added calcium hydride in dry solvent. Hydrogen was evolved and the gas volume was read.

Source and Purity of Materials:

(1) Source not specified; purified by storage over mercury, refluxing with phosphorous pentoxide and fractional distillation; b.p. range 110.4–110.6 °C, (760 Torr).

(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).
Variables:	**Prepared By:**
One temperature: 25 °C	G. T. Hefter

Experimental Data

The solubility of toluene in distilled water at 25 °C was reported to be 506.7 μg/g, corresponding to a mole fraction, x_1, of 5.5 $\cdot 10^{-6}$.

The corresponding mass percent calculated by compiler is 0.0507 $g(1)$/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

500 mL of water and an excess of (1) were equilibrated for at least 24 h in a 1 L Erlenmeyer flask placed in a constant temperature (±0.1 °C) gyrotary shaker (200 rpm). After a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass-wool plug into a calibrated separatory funnel. Toluene was extracted (>99%) by passing known volumes through 0.6×6 cm columns of superficially porous bonded C_{18} stationary-phase adsorbent and eluted with trichlorofluoromethane.

Toluene levels in eluates were determined on an Hewlett-Packard Model 5840A gas chromatograph equipped with a flame ionization detector and a electronic integrator using a 1/8 in 8 ft stainless-steel column of 10% TCPE on 10/120 Chromosorb or WCOTSB-2100 glass column (0.25 mm×30 m).

Hydrocarbon concentrations in eluates were additionally determined by UV spectrophotometry.

Source and Purity of Materials:

(1) Burdick & Jackson; purified by triple distillation in glass.

(2) Doubly distilled in all-glass apparatus; free of trace organics.

Estimated Error:

Temperature: ±0.1 °C.

Solubility: ±6.1 μg/g (standard deviation for 6 determinations).

Components:

(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. Sada, S. Kito, and Y. Ito, J. Chem. Eng. Data **20**, 373 (1975).

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.5633 mL (1)/L (2).

Auxiliary Information

Method/Apparatus/Procedure:

Sudan IV was used to dye (1). The experimental apparatus and procedure used in this work were similar to those of Sobotka and Khan (Ref. 1). To make the measurements more accurate, the apparatus used consisted of a 1 L dissolution flask and a 2 mL microburet. The scale was calibrated in advance by use of mercury. The dissolution flask was immersed in a water bath controlled thermostatically at 25 °C. To avoid condensation of (1) from the gas phase, the temperature of gas phase in the dissolution flask was kept 1 °C higher than that of the liquid phase. The dissolution flask and the microburet were connected tightly.

Source and Purity of Materials:

(1) Source not specified; reagent grade; used as received; purity not specified.
(2) Pure.

Estimated Error:

Temperature: ± 0.01 °C.
Solubility: less than 0.008 mL (1)/L sln (type of error not specified).

References:

[1] H. Sobotka and J. Kahn, J. Am. Chem. Soc. **53**, 2935 (1948).

Components:

(1) Toluene; C_7H_8; [108-88-3]
(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 toluene in water at 25 °C was reported to be $5.65 \cdot 10^{-3}$ mol(1)/L sln.

Assuming a solution density of 1.00 kg/L this corresponds to a solubility of 0.0521 $g(1)$/100 g sln, $x_1 = 1.02 \cdot 10^{-4}$, 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 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:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	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

The solubility of toluene in water

$t/°C$	$10^4 \cdot x_1$ (compiler)	$g(1)/100$ g sln (compiler)[a]	$10^3 \cdot \mathrm{mol}(1)/\mathrm{L}$ sln
15	1.01	0.0514	5.58±0.11
25	1.03	0.0526	5.71±0.14
35	1.07	0.0545	5.88±0.16
45	1.14	0.0584	6.28±0.10

[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 99.0%, 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:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	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 and G. T. Hefter

Experimental Data

Solubility of toluene in water

$t/°C$	$10^4 \cdot x_1$[a]	$g(1)/100$ g sln[a]	$g(1)/\mathrm{L}$ sln
15	1.04	0.0533	0.533±0.017
25	1.09	0.0559	0.557±0.007
35	1.16	0.0590	0.587±0.015
45	1.25	0.0641	0.635±0.019

[a] Assuming the solution density to be that of pure water at the same temperature.[1]

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 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 to 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.

References:

[1] *CRC Handbook of Chemistry and Physics*, R.C. Weast, Editor (CRC Press, Boca Raton, FL, 1982), 63rd ed., pF-11.

Components:

(1) Toluene; C_7H_8; [108-88-3]
(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

Experimentall Values

Solubility of toluene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$5.65\cdot 10^{-3}$	$5.22\cdot 10^{-2}$	$1.021\cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The apparatus used for preparing aqueous solutions saturated with hrocarbon vapor was the same as that previously reported in Sanemasa *et al.*[1] The method was based on the introduction of 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 99%; 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) Toluene; C_7H_8; [108-88-3]
(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 MPa–400 MPa

Prepared By:

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

Experimental Data

Solubility of toluene in water

t/°C	P/MPa	mol (1)/L sln	x_p/x_0	$10^4\cdot g(1)$/100 g sln (compilers)	$10^4\cdot x_1$ (compilers)
25.00	0.1	$6.1\cdot 10^{-3}$	1	5.63	1.10
	50		1.083	6.08	1.19
	100		1.127	6.34	1.24
	150		1.162	6.54	1.28
	200		1.174	6.59	1.29
	250		1.162	6.54	1.28
	300		1.124	6.34	1.24
	350		1.067	6.03	1.18
	400		0.993	5.57	1.09

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 toluene 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 thermoregulated 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 Ref. 1. Solubilities were calculated through the Lambert-Beer's law with use of the molar extinction coefficients. The ratios of solubilities 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, aqueous Na_2CO_3, 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:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	S. Sawamura, K. Nagaoka, and T. Machikawa, J. Phys. Chem. B **105**, 2429 (2001).
Variables: Temperature: 273.2 K–323.2 K Pressure: 0.1 MPa–400 MPa	**Prepared By:** A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

T/K	P/MPa	$g(1)$/100 g sln (compilers)	$10^4 \cdot x_1$
273.2	0.1	0.05828	1.140
278.2	0.1	0.05680	1.111
283.3	0.1	0.05572	1.090
288.2	0.1	0.05521	1.080
293.2	0.1	0.05521	1.080
298.2	0.1	0.05572	1.090
303.2	0.1	0.05731	1.121
308.2	0.1	0.05884	1.151
313.2	0.1	0.06140	1.201
318.2	0.1	0.06395	1.251
323.2	0.1	0.06758	1.322
273.2	25	0.06032	1.180
283.2	25	0.05777	1.130
313.2	25	0.06298	1.232
323.2	25	0.06916	1.353
273.2	50	0.06191	1.211
283.2	50	0.05935	1.161
298.2	50	0.06032	1.180
313.2	50	0.06446	1.261
323.2	50	0.07069	1.383
273.2	75	0.06298	1.232
283.2	75	0.06089	1.191
313.2	75	0.06605	1.292
323.2	75	0.07172	1.403
273.2	100	0.06298	1.232
283.2	100	0.06140	1.201
298.2	100	0.06278	1.228
313.2	100	0.06707	1.312
323.2	100	0.07279	1.424
273.2	150	0.06242	1.221
283.2	150	0.06242	1.221
298.2	150	0.06477	1.267
313.2	150	0.06809	1.332
323.2	150	0.07427	1.453
273.2	200	0.06089	1.191
283.2	200	0.06191	1.211
298.2	200	0.06543	1.280
313.2	200	0.06860	1.342
323.2	200	0.07483	1.464
273.2	250	0.05777	1.130
283.2	250	0.06032	1.180
298.2	250	0.06477	1.267
313.2	250	0.06809	1.332
323.2	250	0.07483	1.464
273.2	300	0.05414	1.059
283.2	300	0.05828	1.140
298.2	300	0.06262	1.225
313.2	300	0.06707	1.312
323.2	300	0.07325	1.433
273.2	350	0.05051	0.988
283.2	350	0.05572	1.090
298.2	350	0.05945	1.163
313.2	350	0.06553	1.282
323.2	350	0.07121	1.393
273.2	400	0.04688	0.917
283.2	400	0.05261	1.029
298.2	400	0.05532	1.082
313.2	400	0.06349	1.242
323.2	400	0.06860	1.342

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Water and a few drops of toluene were placed in a high pressure optical cell with a Teflon ball for stirring as described in Ref. 1. The sample was pressurized and shaken in a thermoregulated water bath for a few days. The absorbance was measured at the absorption maximum around 260 nm. Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1,2]

Solubilities were calculated on the basis of measurements and recommended solubility value at 298.15 K and 0.1 MPa reported in Shaw.[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) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz, Anal. Chem. **52**, 10 (1980).
Variables: One temperature: 23.5 °C	**Prepared By:** M. C. Haulait-Pirson

Experimental Data

Solubility of toluene in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln
23.5	1.31	0.0670±0.0015
23.5	1.29	0.0660±0.0006

Auxiliary Information

Method/Apparatus/Procedure:

An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (∼14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility was calculated from the amount of solute removed from the column, i.e., length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.

Source and Purity of Materials:

(1) 99.9% purity used without further purification.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: ±1.5% (average standard deviation).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz and J. Miller, Anal. Chem. **52**, 2162 (1980).
Variables: Temperature: 10.0 °C–30.0 °C	**Prepared By:** A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

t/°C	$g(1)$/100 g sln	$10^4 \cdot x_1$ (compilers)
10.0[a]	0.0758±0.0010	1.483
10.0[b]	0.0777±0.0010	1.520
20.0[a]	0.0732±0.0020	1.432
20.0[b]	0.0739±0.0010	1.446
30.0[a]	0.0920±0.0002	1.800
30.0[b]	0.0754±0.0010	1.475

Auxiliary Information

Method/Apparatus/Procedure:

Two methods (a) the elution chromatography method, described in Schwarz[1] and (b) the UV absorption method, were used. For (a) 3 mm o. d. columns ∼25 cm long and containing 0.3–0.5 g of solute were used. The measurement time was 1–14 days. Each solubility was determined from 2 different columns. For (b) a solution obtained in an equilibrium apparatus was diluted with ethanol, UV absorption measurements were performed and compared with solutions of known composition. Each solubility was determined twice. Details of the apparatus, and procedures were described in the paper.

Source and Purity of Materials:

(1) Source not specified; purity 99.9 mass %; used as received.
(2) Distilled water.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: as above.

References:

[1] F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).
Variables:	**Prepared By:**
Temperature: 0 °C–90.2 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

t/°C	$10^3 \cdot g(1)$/100 g sln	$10^4 \cdot x_1$ (compilers)
0.0	0.12	2.3
9.5	0.09	1.8
19.8	0.08	1.6
25.0[a]	0.053	1.0
29.7	0.08	1.6
39.6	0.10	2.0
40.0[a]	0.06	1.2
50.0	0.09	1.8
60.1	0.10	2.0
70.4	0.09	1.8
81.0	0.13	2.5
90.2	0.12	2.3

[a] Part of ternary solubility measurements.

Solubility of water in toluene

t/°C	$g(2)$/100 g sln	$10^3 \cdot x_2$ (compilers)
0.0	0.042	0.21
9.5	0.057	0.29
19.8	0.087	0.44
25.0[a]	0.060	0.31
29.7	0.092	0.47
39.6	0.110	0.56
40.0[a]	0.110	0.56
50.0	0.140	0.71
60.1	0.151	0.77
70.4	0.206	1.04
81.0	0.247	1.25
90.2	0.281	1.42

[a] Part of ternary solubility measurements.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Toluene (1) and water (2) were brought into equilibrium at a given temperature in a thermostat, and samples of each layer were removed by syringe for analysis. To each sample a higher boiling organic compound was added as a standard and the ratio of peaks was measured by gas chromatography, Stephenson *et al.*[1,2] Temperature was measured by a calibrated thermometer accurate to 0.1 °C.

Source and Purity of Materials:

(1) Aldrich Chemical Co.; purity >99.9 mass %.
(2) Not stated.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: std deviation: 0.01 and 0.005 g/100 g sln in toluene-rich phase and water-rich phase, respectively.

References:

[1] R. M. Stephenson, J. Stuart, and M. Tabak, J. Chem. Eng. Data **29**, 287 (1984).
[2] R. M. Stephenson and J. Stuart, J. Chem. Eng. Data **31,** 56 (1986).

Components:
(1) Toluene; C_7H_8; [108-88-3]
(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 toluene in water at 25 °C was reported to be 534.8 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.05348 $g(1)/100$ g sln and $1.046 \cdot 10^{-4}$.

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: 4.9 mg (1)/kg (2) (standard deviation of the mean for six replicates).

Components:
(1) Toluene; C_7H_8; [108-88-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
K. Tamura, Y. Chen, and T. Yamada, J. Chem. Eng. Data **46**, 1381 (2001).

Variables:
One temperature: 298.15 K

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

Experimental Data

Solubility of water in toluene

t/K	$g(2)/100$ g sln (compilers)	x_2
298.15	0.00092	0.0047

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The experimental apparatus and procedure were described in Tamura *et al.*[1] The sample mixtures, withdrawn from upper and lower phases in equilibrium were analyzed by glc (Shimadzu GC-8A apparatus equipped with a thermal conductivity detector, 2 m stainless steel column with Porapak SQ; He flow rate 0.5 cm^3/s; temperature of the injection port and detector −463.15 K; temperature of the oven: initial −424 K, final −493 K, rate −32 K/min.). A mean value of at least 3 analyses was reported.

Reported data were from a study of the ternary toluene-water-methanol system.

Source and Purity of Materials:
(1) Aldrich Chemical Co., purity 99.8 mass %; purity >99.8 mass % checked by glc; ρ^{25} 0.86235; used as received.
(2) Wako Pure Chemical, purity 99.9 mass %; ρ^{25} 0.99692.

Estimated Error:
Solubility: ±0.001 mole fraction (authors).

References:
[1] K. Tamura, Y. Chen, K. Tada, and T. Yamada, Fluid Phase Equlib. **171**, 115 (2000).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	D. N. Tarassenkow and E. N. Poloshinzewa, Ber. Dtsch. Chem. Ges., B **65**, 184 (1932).
Variables: Temperature: (-9) °C–93 °C	**Prepared By:** A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in toluene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
-9	0.1	0.002
-3.5	0.3	0.005
10.5	1.0	0.020
18	1.7	0.034
30	2.7	0.053
38.5	3.6	0.070
48	4.9	0.097
60.5	7.8	0.153
68	10.2	0.201
76	12.9	0.254
84	15.8	0.312
93	20.8	0.413

Auxiliary Information

Method/Apparatus/Procedure:

Alexejew's method was used (Alexejew[1]). No additional details were reported in the paper.

Source and Purity of Materials:

(1) Kahlbaum, CP; dried over calcium chloride and distilled from sodium; purity not specified.
(2) Not specified.

Estimated Error:

Solubility: ±0.01% (not specified).

References:

[1] W. Alexejew, Wied Ann. Physik **28**, 35 (1886).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (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: One temperature: 25.0 °C	**Prepared By:** A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$6.28 \cdot 10^{-3}$	$5.81 \cdot 10^{-2}$	$1.135 \cdot 10^{-4}$

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 was 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. De Voe, 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:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	S. P. Uspenskii, Neft. Khoz. **11–12**, 713 (1929).

Variables:	**Prepared By:**
Temperature: 10 °C and 22 °C	A. Maczynski and Z. Maczynska

Experimental Data

Solubility of toluene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln
10	7.20	0.0368±0.0002
22	9.62	0.0492±0.0003

Solubility of water in toluene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	2.18	0.0426±0.0011
22	2.68	0.0526±0.0016

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by titration. The solubility of (2) in (1) was determined by Clifford's (Clifford[1]) method. Dried air was passed through the vessel with a saturated solution of (2) in (1) and U-tubes with $CaCl_2$, and next absorbed (2) was weighed.

Source and Purity of Materials:

(1) Source not specified; boiling point 109.8 °C at 752 mmHg, $d_4^{22}=0.8636$, and $d_4^{10}=0.8743$.
(2) Not specified.

Estimated Error:

Solubility: see experimental values above.

References:

[1] C. W.Clifford, Ind. Eng. Chem. **13**, 628 (1921).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

Variables:	**Prepared By:**
One temperature: 298.15 K	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of toluene in water

T/K	mol (1)/g (2)	$g(1)$/100 g sln (compilers)	x_1 (compilers)
298.15	$(6.81\pm0.08)\cdot10^{-6}$	$6.27\cdot10^{-4}$	$1.226\cdot10^{-4}$

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. Temperature was maintained within ±0.05 K by means of a water bath. 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).

Components:	Original Measurements:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	J. Wing and W. H. Johnston, J. Am. Chem. Soc. **79**, 864 (1957).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in toluene at 25 °C was reported to be 0.0334 mL (2)/100 mL sln.

Auxiliary Information

Method/Apparatus/Procedure:

A small amount of (2) was equilibrated with 20 mL of (1) using a Teflon stirrer in a 100 mL flask in a Sargent constant temperature bath. At the end of 2 h, the mixture was poured into a test tube immersed in the bath and the organic phase separated from water by gravity. The determination of THO in the organic phase was done by isotopic dilution with a large excess of H_2O. The tritium activities in the tritiated water samples were determined by the acetylene method described in Wing and Johnson.[1]

Source and Purity of Materials:

(1) Source not specified, chemical grade; redistilled in a column of 50 theoretical plates; purity not specified.
(2) Tracerlab, Inc., tritiated water with an activity of approximately 1 μCi/mL.

Estimated Error:

Temperature: ±0.02 °C.
Solubility: 0.8% (standard deviation from 5 determinations).

References:

[1] J. Wing and W. H. Johnson, Science **121**, 674 (1955).

2.5. Toluene+Heavy Water

Components:	Original Measurements:
(1) Toluene; C_7H_8; [108-88-3] (2) Heavy water (deuterium oxide); D_2O; [7789-20-0]	P. K. Glasoe and S. D. Schultz, J. Chem. Eng. Data **17**, 66 (1972).
Variables:	**Prepared By:**
Temperature: 15 °C–30 °C	A. Maczynski and Z. Maczynska

Experimental Data

Solubility of heavy water in toluene

$t/°C$	$10^3 \cdot x_2$ (compiler)	$g(2)/100$ g sln (compiler)	mol (2)/L sln
15	1.71	0.0372	0.0162
25	2.31	0.0504	0.0213
30	2.57	0.0560	0.0240

The compilers' calculations assume a solution density of 0.862 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

Dried (1) was saturated with (2) by allowing it to stand in contact with (2) in a closed system, protected from atmospheric moisture.
This two-phase system was kept in a pyrex storage bottle which was immersed in a constant temperature water bath.

The concentration of (2) in (1) was determined by the Karl Fischer method.

Source and Purity of Materials:

(1) Source not specified; reagent grade; purified by distillation and dried over molecular sieve.
(2) Distilled in a pyrex system.

Estimated Error:

Solubility: ±0.0004 mol(2)/L sln (type of error not specified).

Components:	**Original Measurements:**
(1) Toluene; C_7H_8; [108-88-3] (2) Heavy water (deuterium oxide); D_2O; [7789-20-0]	A. N. Guseva and E. I. Parnov, Radiokhimiya **5**, 507 (1963).
Variables: Temperature: 87 °C–203 °C	**Prepared By:** A. Maczynski

Experimental Data

Solubility of toluene in heavy water

t/°C	$10^3 \cdot x_1$	$g(1)$/100 g sln (compiler)
87	0.682	0.313
123	1.81	0.828
164.5	4.22	1.91
203	7.51	3.37

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in Khazanov.[1]

Source and Purity of Materials:

(1) Not specified.
(2) Distilled.

Estimated Error:

Not specified.

References:

[1] P. E. Khazanova, Tr. Gos. Inst. Azotn. Promyshl. **4**, 5 (1954).

2.6. Cycloheptene+Water

Components:	**Original Measurements:**
(1) Cycloheptene; C_7H_{12}; [628-92-2] (2) Water; H_2O; [7732-18-5]	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 cycloheptene in water at 25 °C was reported to be 66 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0066 $g(1)$/100 g sln and $1.2 \cdot 10^{-5}$.

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. 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 conjunction 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) (standard deviation of mean).

2.7. 1,6-Heptadiene+Water

Components:

(1) 1,6-Heptadiene; C_7H_{12} ; [3070-53-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of 1,6-heptadiene in water at 25 °C was reported to be 44 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.0044 $g(1)/100$ g sln and $8.2\cdot 10^{-6}$.

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. 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 conjunction 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: 3 mg (1)/kg (2) (standard deviation of mean).

2.8. 1-Heptyne+Water

Components:

(1) 1-Heptyne; C_7H_{12} ; [628-71-7]
(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-heptyne in water at 25 °C was reported to be 94 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.0094 $g(1)/100$ g sln and $1.76\cdot 10^{-5}$.

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. 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 conjunction 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: 3 mg (1)/kg (2) (standard deviation of mean).

2.9. 1-Methylcyclohexene+Water

Components:
(1) 1-Methylcyclohexene; C_7H_{12} ; [591-49-1]
(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-methylcyclohexene in water at 25 °C was reported to be 52 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.0052 $g(1)/100\ g\ sln$ and $9.7\cdot 10^{-6}$.

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. 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 conjunction 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: 52 mg (1)/kg (2) (standard deviation of mean).

2.10. Cycloheptane+Water

Components:
(1) Cycloheptane; C_7H_{14} ; [291-64-5]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

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

The experimental solubility data for (1) in (2) have been investigated by Groves[1] at 303 K, and McAuliffe[2] at 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:

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

where $\ln x_{\min,1} = -12.45$, $\Delta_{\mathrm{sln}} C_p / R = 42.6$, and $T_{\min} = 298$ K.

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

All the experimental and reference data are listed in Table 7. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:
[1] F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).
[2] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

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

T/K	Experimental values x_1 (T=tentative)	Reference values $x_1 \pm 30\%$
298.2	$5.50\cdot 10^{-6}$ (T; Ref. 2)	$4.3\cdot 10^{-6}$
303.2	$4.99\cdot 10^{-6}$ (T; Ref. 1)	$4.3\cdot 10^{-6}$

Components:

(1) Cycloheptane; C_7H_{14}; [291-64-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).

Variables:

One temperature: 30.0 °C

Prepared By:

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

Experimental Data

Solubility of cycloheptane in water

$t/°C$	mg (1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
30.0	27.1 ± 1.4	0.00272	$4.99 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method, similar to that used in Polak and Liu,[1] was used. Hydrocarbon (1) was injected into a 40 mL vial fitted with a Teflon-lined septum and containing about 20 mL water. Following an equilibration period of 2 weeks in a thermostatted, the water layer was analyzed chromatographically (3% SP-1500 on Carbopack B at 150 °C, He carrier gas at 30 mL/min., FID detector). The reported result is average of four replicate determinations.

Source and Purity of Materials:

(1) Aldrich, Chemical Co.; purity 98%; used as received.
(2) Distilled.

Estimated Error:

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

References:

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

Components:

(1) Cycloheptane; C_7H_{14}; [291-64-5]
(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 cycloheptane in water at 25 °C was reported to be 30 mg (1)/kg sln [0.0030 $g(1)/100$ g sln].

The corresponding mole fraction, x_1, calculated by the compiler, is $5.5 \cdot 10^{-6}$. 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 μL sample of the (1) saturated water was withdrawn with a Hamilton syringe and injected into a 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: 1.0 mg (1)/kg sln (standard deviation of mean).

References:

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

2.11. Ethylcyclopentane+Water

Components:

(1) Ethylcyclopentane; C_7H_{14} ; [1640-89-7]
(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 ethylcyclopentane

$t/°C$	$10^4 \cdot x_2$ (compiler)	$g(2)/100$ g sln
10	3.87	0.0071
20	6.49	0.0119
30	10.14	0.0186

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) Ethylcyclopentane; C_7H_{14} ; [1640-89-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).

Variables:

Temperature: 70.5 °C–203 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Data

Solubility of ethylcyclopentane in water

$t/°C$	$10^4 \cdot x_1$ (compiler)	$g(1)/100$ g sln	$g(1)/100$ g sln (compiler)
70.5	0.40	0.0219	0.0219
113	0.96	0.0525	0.0525
168.5	4.10	0.224	0.224
203	13.89	0.759	0.759

Auxiliary Information

Method/Apparatus/Procedure:

Presumably the measurements were made in sealed glass tubes, as reported in Guseva and Pamov.[1] No more details were reported in the paper.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

References:

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

2.12. 1-Heptene+Water

Components:	**Evaluators:**
(1) 1-Heptene; C_7H_{14} ; [592-76-7] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

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

The experimental solubility data for (1) in (2) have been investigated by Natarajan and Venkatachalam[3] at 293 K–303 K and Tewari *et al.*[4] at 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:

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

where $\ln x_{1,\min} = -12.94$, $\Delta_{\text{sln}} C_p / R = 51.3$, 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.

The experimental and reference data of Natarajan and Venkatachalam[3] and Tewari *et al.*[4] are listed in Table 8. The data of Natarajan and Venkatachalam[3] and Tewari *et al.*[4] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

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

The experimental solubility data for (1) in (2) have been investigated by Black *et al.*[1] at 283 K–294 K and Englin *et al.*[2] at 283 K–303 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:

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

where $d_1 = -1.090$, $d_2 = -2.642$, $d_3 = 1.406$, $d_4 = -10.413$, and $T_r = T/522.1$.

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-heptene 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 9. The data of Englin *et al.*[2] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Black *et al.*[1] are in poor agreement with the reference data and are Doubtful.

References:

[1] C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).

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

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

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

TABLE 8. Experimental values for solubility of 1-heptene (1) in water (2)

T/K	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
293.2	$5.70 \cdot 10^{-6}$ (D; Ref. 3)	$2.5 \cdot 10^{-6}$
298.2	$5.10 \cdot 10^{-6}$ (D; Ref. 3)	$2.4 \cdot 10^{-6}$
298.2	$3.34 \cdot 10^{-6}$ (D; Ref. 4)	$2.4 \cdot 10^{-6}$
303.2	$4.40 \cdot 10^{-6}$ (D; Ref. 3)	$2.4 \cdot 10^{-6}$

TABLE 9. Experimental values for solubility of water (2) in 1-heptene (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
283.2	$3.76 \cdot 10^{-3}$ (D; Ref. 1), $1.01 \cdot 10^{-3}$ (T; Ref. 2)	$9.1 \cdot 10^{-4}$
293.2	$1.36 \cdot 10^{-3}$ (T; Ref. 2)	$1.3 \cdot 10^{-3}$
293.3	$6.11 \cdot 10^{-3}$ (D; Ref. 1)	$1.3 \cdot 10^{-3}$
293.7	$5.68 \cdot 10^{-3}$ (D; Ref. 1)	$1.3 \cdot 10^{-3}$
294.4	$6.28 \cdot 10^{-3}$ (D; Ref. 1)	$1.3 \cdot 10^{-3}$
303.2	$2.04 \cdot 10^{-3}$ (T; Ref. 2)	$1.8 \cdot 10^{-3}$

Components:

(1) 1-Heptene; C_7H_{14} ; [592-76-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).

Variables:

Temperature: 10 °C–21.2 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in 1-heptene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g (1)
10.0	3.76	0.0692
20.1	6.11	0.1126
20.5	5.68	0.1047
21.2	6.28	0.1158

At total saturation pressure of 1 atm.

Auxiliary Information

Method/Apparatus/Procedure:

Air-saturated with radioactive water vapor was bubbled through (1) until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred to a scintillation counter by equilibration with ethanol vapor. The method is described in Joris and Taylor.[1]

Source and Purity of Materials:

(1) Harvard University; purity not specified; used as received.
(2) Not specified.

Estimated Error:

Solubility: ±1% (type of error not specified).

References:

[1] G. G. Joris and H. S. Taylor, J. Chem Phys. **16**, 45 (1948)

Components:

(1) 1-Heptene; C_7H_{14} ; [592-76-7]
(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 Z. Maczynska

Experimental Data

Solubility of water in 1-heptene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	1.01	0.0186
20	1.36	0.0249
30	2.04	0.0375

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) 1-Heptene; C_7H_{14} ; [592-76-7] (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 1-heptene in water

$T/°C$	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$1.85 \cdot 10^{-4}$	$1.82 \cdot 10^{-3}$	$3.34 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used, 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. De Voe, 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:	Original Measurements:
(1) 1-Heptene; C_7H_{14} ; [592-76-7] (2) Water; H_2O; [7732-18-5]	G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).
Variables:	**Prepared By:**
Temperature: 20 °C–30 °C	M. C. Haulait-Pirson and G. T. Hefter

Experimental Data

Solubility of 1-heptene in 0.001 mol·/L HNO_3 solution

$t/°C$	$10^6 \cdot x_1$ (compiler)	$10^3 \cdot g(1)$/100 g sln[b] (compiler)	$10^4 \cdot$ mol(1)/L sln[a]
20	5.7	3.1	3.16 ± 0.13
25	5.1	2.8	2.81 ± 0.12
30	4.4	2.4	2.45 ± 0.15

[a] Uncertainties stated to be "standard deviations from means."
[b] Assuming a solution density of 1.00 g mL^{-1} at all temperatures.

Compiler's note: Although the data have not been measured in pure water the low concentration of the added acids is unlikely to cause the solubility to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol·/L HCl.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Matheson, Coleman and Bell; 99%.
(2) Not specified.

Estimated Error:

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

2.13. 2-Heptene+Water

Components:
(1) 2-Heptene; C_7H_{14}; [592-77-8]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

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

The experimental solubility data for (1) in (2) have been investigated by McAuliffe[1] and Natarajan and Venkatachalam[2] at 298 K, and Schwarz[3] at 297 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:

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

where $\ln x_{1,\min} = -12.54$, $\Delta_{\mathrm{sln}} C_p / R = 49.3$, 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.

The experimental and reference data of McAuliffe,[1] Natarajan and Venkatachalam,[2] and Schwarz[3] are listed in Table 10. The data of McAuliffe[1] and Schwarz[3] are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Natarajan and Venkatachalam[2] are in poor agreement with the reference data and are Doubtful.

References:

[1] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[2] G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).
[3] F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

TABLE 10. Experimental values for solubility of 2-heptene (1) in water (2)

T/K	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
296.7	$2.75 \cdot 10^{-6}$ (T; Ref. 3)	$3.7 \cdot 10^{-6}$
298.2	$2.70 \cdot 10^{-6}$ (T; Ref. 1), $4.89 \cdot 10^{-6}$ (D; Ref. 2)	$3.6 \cdot 10^{-6}$

Components:
(1) 2-Heptene; C_7H_{14}; [592-77-8]
(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 2-heptane in water at 25 °C was reported to be 15 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0015 *g* (1)/100 g sln and $2.7 \cdot 10^{-6}$.

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. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton Syringe and gas liquid chromatographed in conjunction 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: 1.4 mg (1)/kg (2) (standard deviation of mean).

Components:

(1) 2-Heptene; C_7H_{14} ; [592-77-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Variables:

One temperature: 23.5 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Data

The solubility of 2-heptane in water at 23.5 °C was reported to be 0.00150 ± 0.00003 g (1)/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compiler is $2.75 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

An elusion chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (Chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (~14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e., length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.

Source and Purity of Materials:

(1) 99% purity used without further purification.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 2% (average standard deviation).

Components:

(1) 2-Heptene; C_7H_{14} ; [592-77-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson and G. T. Hefter

Experimental Data

The solubility of 2-heptane in water was reported to be $2.716 \cdot 10^{-4}$ mol·/L at 25 °C.[a]

Assuming a solution density of 1.00 g·/mL the corresponding mass percent and mole fraction, x_1 , solubilities, calculated by the compilers are, respectively, 0.00266 $g(1)$/100 g sln and $4.89 \cdot 10^{-6}$.

Solubility data are also presented as a function of temperature in various salt solutions.

[a] It should be noted that although the authors state that the solubility refers to ‘‘water’’ the context in the paper is ambiguous and the data were probably obtained in 0.001 mol·/L HNO_3 solution.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Prepared by dehydration of 2-heptanol and then washed, dried, and fractionated; purity (no specification) was determined by chromatography.
(2) Not specified.

Estimated Error:

Temperature: ±0.05 °C.
Solubility: not specified.

2.14. Methylcyclohexane+Water

Components:	**Evaluators:**
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

Critical Evaluation of the Solubility of Methylcyclohexane (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
Groves[2]	298	McAuliffe[5]	298
Guseva and Parnov[3]	341–488	Price[6]	298–423
Hellinger and Sandler[4]	298	Rudakov and Lutsyk[7]	298

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

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

where $\ln x_{\mathrm{min},1} = -12.85$, $\Delta_{\mathrm{sln}} C_p / R = 44.7$, and $T_{\mathrm{min}} = 298$ K.

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

All the experimental and reference data are listed in Table 11 and shown in Fig. 5. The data of Groves,[2] Price,[6] and Rudakov and Lutsyk[7] at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. The data of Hellinger and Sandler,[4] and McAuliffe[5] at 298 K, and Price[6] at 313 K–410 K are in good agreement with the reference data and are Tentative. The data of Guseva and Parnov[3] at 341 K–488 K and Price[6] at 423 K are in poor agreement with the reference data and are Doubtful.

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

The experimental solubility data for (2) in (1) have been investigated by Englin *et al.*[1] at 273 K–303 K, and Hellinger and Sandler[4] 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:

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

where $d_1 = -0.203$, $d_2 = -6.277$, $d_3 = -1.935$, $d_4 = -1.695$, and $T_r = T/545.3$.

Equation (2) was used for obtaining Reference data by regression of the data obtained from those calculated from Reference data of solubility of methylcyclohexane 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. All the data are in poor agreement with the reference data and are Doubtful.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[8] are independent data.

References:

[1] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[2] F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).
[3] A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).
[4] S. Hellinger and S. I. Sandler, J. Chem. Eng. Data **40**, 321 (1995).
[5] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[6] L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[7] E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).
[8] T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

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

T/K	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
298.2	$3.07\cdot10^{-6}$ (R; Ref. 2), $2.33\cdot10^{-6}$(T; Ref. 4), $2.62\cdot10^{-6}$(T; Ref. 4), $2.60\cdot10^{-6}$(T; Ref. 5), $2.90\cdot10^{-6}$(R; Ref. 6), $2.70\cdot10^{-6}$(R; Ref. 7)	$2.9\cdot10^{-6}$
313.3	$3.30\cdot10^{-6}$ (T; Ref. 6)	$3.1\cdot10^{-6}$
328.9	$3.50\cdot10^{-6}$ (T; Ref. 6)	$3.6\cdot10^{-6}$
341.2	$2.00\cdot10^{-5}$ (D; Ref. 3)	$4.3\cdot10^{-6}$
372.3	$6.20\cdot10^{-6}$ (T; Ref. 6)	$8.1\cdot10^{-6}$
393.2	$1.46\cdot10^{-5}$ (T; Ref. 6)	$1.4\cdot10^{-5}$
393.7	$6.70\cdot10^{-5}$ (D; Ref. 3)	$1.4\cdot10^{-5}$
410.5	$2.55\cdot10^{-5}$ (T; Ref. 6)	$2.3\cdot10^{-5}$
422.7	$4.48\cdot10^{-5}$ (D; Ref. 6)	$3.3\cdot10^{-5}$
430.7	$1.71\cdot10^{-4}$ (D; Ref. 3)	$4.3\cdot10^{-5}$
488.2	$1.39\cdot10^{-3}$ (D; Ref. 3)	$3.0\cdot10^{-4}$

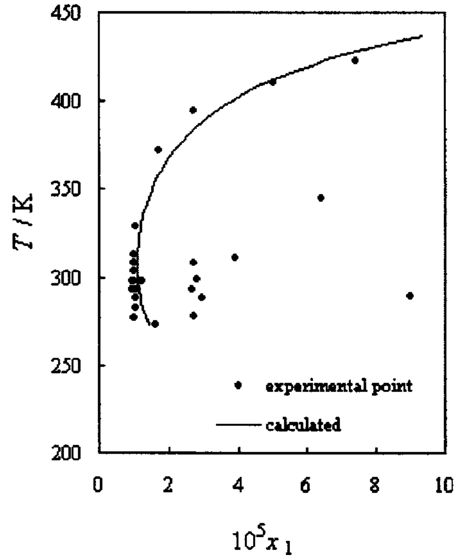

FIG. 5. All the solubility data for methylcyclohexane (1) in water (2).

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

T/K	Experimental values x_2 (D=doubtful)	Reference values $x_2 \pm 30\%$
283.2	$3.33\cdot10^{-4}$ (D; Ref. 1)	$2.4\cdot10^{-4}$
293.2	$6.32\cdot10^{-4}$ (D; Ref. 1)	$3.8\cdot10^{-4}$
298.2	$1.92\cdot10^{-3}$ (D; Ref. 4), $9.2\cdot10^{-4}$ (D; Ref. 4)	$4.7\cdot10^{-4}$
303.2	$9.75\cdot10^{-4}$ (D; Ref. 1)	$5.8\cdot10^{-4}$

Components:	**Original Measurements:**
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (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 methylcyclohexane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.33	0.0061
20	6.32	0.0116
30	9.75	0.0179

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of methylcyclohexane in water

t/°C	mg (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	16.7±0.6	0.00167	$3.07 \cdot 10^{-6}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method, similar to that mentioned in Polak and Liu,[1] was used. Hydrocarbon (1) was injected into 40 mL vials fitted with Teflon-lined septa containing about 20 mL water and placed in a thermostatted bath for 2 weeks. The water layer was analyzed chromatographically (3% SP-1500 on Carbopack B at 150 °C, He carrier gas at 30 mL/min, FID detector). The reported result is the mean of four replicate determinations.

Source and Purity of Materials:

(1) Aldrich, Chemical Co.; purity 99%; used as received.
(2) Distilled.

Estimated Error:

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

References:

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

Components:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).

Variables:
Temperature: 68 °C–215 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of methylcyclohexane in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln	$g(1)$/100 g sln (compiler)
68	0.20	0.011	0.011
120.5	0.67	0.0363	0.0363
157.5	1.71	0.0933	0.0933
215	13.90	0.759	0.759

Auxiliary Information

Method/Apparatus/Procedure:

Presumably the measurements were made in sealed glass tubes, as reported in Guseva and Pamov.[1] No more details were reported in the paper

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

Estimated Error:
Not specified.

References:

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

Components:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Hellinger and S. I. Sandler, J. Chem. Eng. Data **40**, 321 (1995).

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of methylcyclohexane in water

t/°C	$10^3 \cdot g(1)$/100 g sln (compilers)	$10^6 \cdot x_1$
25.0	1.27	2.33
	1.43	2.62

Solubility of water in methylcyclohexane

t/°C	$10^2 \cdot g(2)$/100 g sln (compilers)	$10^3 \cdot x_2$
25.0	3.53	1.92
	1.51	0.82

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:
(1) Aldrich Chemicals Co.; purity 99%; used as received.
(2) Deionized with Barnstead NANO pure equipment.

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

References:

[1] T. Magnussen, P. Rasmussen, and Aa. Fredenslund, Ind. Eng. Chem. Process Des. Deviation **20**, 331 (1981).

[2] C. McAuliffe, Nature (London) **200**, 1002 (1963).

Components:

(1) Methylcyclohexane; C_7H_{14}; [108-87-2]
(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 methylcyclohexane in water at 25 °C was reported to be 14 mg(1)/kg sln[0.0014 $g(1)/100$ g sln].

The corresponding mole fraction, x_1, calculated by the compiler, is $2.6 \cdot 10^{-6}$. The same value is also reported in the two publications by McAuliffe.[1,2]

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 μL sample of the (1) saturated water was withdrawn with a Hamilton syringe and injected into the fractionator of 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: 1.2 mg (1)/kg sln (standard deviation of mean).

References:

[1] C. McAuliffe, Nature (London) **200**, 1092 (1963).
[2] C. McAuliffe, Am. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

Components:

(1) Methylcyclohexane; C_7H_{14}; [108-87-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 25 °C–149.5 °C

Prepared By:

F. Kapuku

Experimental Data

Solubility of methylcyclohexane in water at system pressure

$t/°C$	$10^6 \cdot x_1$ (compiler)	$g(1)/100$ g sln (compiler)	mg (1)/kg (2)
25.0	2.9	0.00160	16.0±0.2
40.1	3.3	0.00180	18.0±0.6
55.7	3.5	0.00189	18.9±0.5
99.1	6.2	0.00338	33.8±1.0
120.0	14.6	0.00795	79.5±2.2
137.3	25.5	0.01390	139.0±8.0
149.5	44.8	0.02440	244.0±10.0

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 obtained 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:	**Original Measurements:**
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Data

The authors reported the partition coefficient α of methylcyclohexane between the gas and aqueous phase. $\alpha = 16 \pm 1$. $\alpha = C_g / C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25 °C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of P (where P is the vapor pressure in mm of Hg) is taken from Hine and Mooker.[1] $P = 46.33$ mm of Hg and $\log C_g = \log P - 4.269 = -2.60$ expressed in moles per liter. Therefore $C_s = 1.56 \cdot 10^{-4}$ moles/L.

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent is 0.0015 $g(1)/100$ g sln and the corresponding mole fraction, x_1, is $2.7 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.

Source and Purity of Materials:

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

Estimated Error:

Solubility: ±10% (estimated by the compiler).

References:

[1] J. Hine and P. K. Mooker, Org. Chem. **4**, 292 (1975).

2.15. 2,2-Dimethylpentane+Water

Components:	**Original Measurements:**
(1) 2,2-Dimethylpentane; C_7H_{16}; [590-35-2] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Data

The solubility of 2,2-dimethylpentane in water at 25 °C and at system pressure was reported to be 4.40 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $4.4 \cdot 10^{-4}$ $g(1)/100$ g sln and $7.9 \cdot 10^{-7}$.

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: ±0.11 mg(1)/kg(2).

2.16. 2,3-Dimethylpentane+Water

Components:	**Original Measurements:**
(1) 2,3-Dimethylpentane; C_7H_{16}; [565-59-3] (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 2,3-dimethylpentane in water at 25 °C and at system pressure was reported to be 5.25 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $5.25\cdot 10^{-4}$ g(1)/100 g sln and $9.43\cdot 10^{-7}$.

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: ±0.02 mg(1)/kg(2).

2.17. 2,4-Dimethylpentane+Water

Components:	**Evaluators:**
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

Critical Evaluation of the Solubility of 2,4-Dimethylpentane (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
McAuliffe[1]	298	Polak and Lu[3]	273 and 298
McAuliffe[2]	298	Price[4]	298

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

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

where $\ln x_{\min,1} = -14.16$, $\Delta_{\text{sln}}C_p/R = 51.4$, and $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of 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. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

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

The experimental solubility data for (2) in (1) have been investigated only by Polak and Lu[3] at 273 K 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:

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

where $d_1 = -0.974$, $d_2 = -6.061$, $d_3 = -0.081$, $d_4 = -4.808$, and $T_r = T/509.3$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of 2,4-dimethylpentane 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.

All the experimental and reference solubility data for (2) in (1) are listed in Table 14. The data of Polak and Lu[3] at 273 K, are in good agreement with the reference data and are Tentative. The remaining data at 298 K are in poor agreement with the reference data and are Doubtful.

Rejected and Inaccessible Data

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

References:

[1] C. McAuliffe, Nature (London) **200**, 1092 (1963).

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

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

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

[5] T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

TABLE 13. Experimental values for solubility of 2,4-dimethylpentane (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative)	Reference values $x_1 \pm 30\%$
273.2	$1.17\cdot 10^{-6}$ (T; Ref. 3)	$1.1\cdot 10^{-6}$
298.2	$6.50\cdot 10^{-7}$ (T; Ref. 1), $7.30\cdot 10^{-7}$ (T; Ref. 2), $9.88\cdot 10^{-7}$ (T; Ref. 3), $7.92\cdot 10^{-7}$ (T; Ref. 4)	$8.0\cdot 10^{-7}$

TABLE 14. Experimental values for solubility of water (2) in 2,4-dimethylpentane (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2	$1.73 \cdot 10^{-4}$ (T; Ref. 3)	$2.0 \cdot 10^{-4}$
298.2	$4.51 \cdot 10^{-4}$ (D; Ref. 3)	$6.6 \cdot 10^{-4}$

Components: (1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	**Original Measurements:** C. McAuliffe, Nature (London) **200**, 1092 (1963).
Variables: One temperature: 25 °C	**Prepared By:** M. C. Haulait-Pirson

Experimental Data

The solubility of 2,4-dimethylpentane in water at 25 °C was reported to be 3.62 mg(1)/kg sln[0.00362 $g(1)$/100 g sln]. The corresponding mole fraction, x_1, calculated by the compiler, is $6.5 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

20–50 mL of (1) was added to (2) and vigorously shaken or stirred several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was directly injected into a gas chromatograph fitted with a suitable fractionator to absorb water. A hydrogen-flame ionization detector was used.

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 0.10 mg (1)/kg sln (standard deviation from mean).

Components:

(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7]
(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 2,4-dimethylpentane in water at 25 °C was reported to be 4.06 mg (1)/kg sln [0.00406 $g(1)$/100 g sln]. The corresponding mole fraction, x_1, calculated by the compiler, is $7.3\cdot 10^{-7}$. 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 μL sample of the (1) saturated water was withdrawn with a Hamilton syringe and injected into the fractionator of 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: 0.29 mg (1)/kg sln (standard deviation of mean).

References:

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

Components:

(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7]
(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 2,4-dimethylpentane in water

t/°C	x_1 (compiler)	mg (1)/kg sln
0[a]	$1.17\cdot 10^{-6}$	6.50[c]
25[b]	$9.88\cdot 10^{-7}$	5.50[c]

Solubility of water in 2,4-dimethylpentane

t/°C	x_2 (compiler)	mg (2)/kg sln
0[a]	$1.73\cdot 10^{-4}$	31[d]
25[b]	$4.51\cdot 10^{-4}$	81[e]

[a–e] See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

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) ±1.7%; (d) ±4.7%; (e) ±3.1 (mean).

Components:	**Original Measurements:**
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (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 2,4-dimethylpentane in water at 25 °C and at system pressure was reported to be 4.41 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $4.41\cdot 10^{-4}$ $g(1)/100$ g sln and $7.92\cdot 10^{-7}$.

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).

2.18. 3,3-Dimethylpentane+Water

Components:	**Original Measurements:**
(1) 3,3-Dimethylpentane; C_7H_{16}; [562-49-2] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
Temperature: 25 °C–150.4 °C	F. Kapuku

Experimental Data

Solubility of 3.3-dimethylpentane in water at system pressure

$t/°C$	$10^6\cdot x_1$ (compiler)	$g(1)/100$ g sln (compiler)	mg (1)/kg (2)
25.0	1.06	0.000592	5.92±0.06
40.1	1.22	0.000678	6.78±0.20
55.7	1.47	0.000817	8.17±0.46
69.7	1.85	0.00103	10.3±0.7
99.1	2.84	0.00158	15.8±0.7
118.0	4.91	0.00273	27.3±0.4
140.4	12.10	0.00673	67.3±1.7
150.4	15.48	0.00861	86.1±1.8

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 the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear 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.

2.19. Heptane+Water

Components:	Evaluators:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

Critical Evaluation of the Solubility of Heptane (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
Bittrich *et al.*[1]	298 and 313	Krasnoshchekova and Gubergrits[13]	298
Booth and Everson[3]	298	McAuliffe[14]	298
Budantseva *et al.*[4]	293 and 313	McCants *et al.*[15]	311
Durand[6]	289	Nelson and De Ligny[16]	277–318
Fühner[8]	289	Polak and Lu[17]	273 and 298
Guseva and Parnov[10]	345–460	Price[18]	298–424
Jonsson *et al.*[11]	288–308	Rudakov and Lutsyk[19]	298
Korenman and Aref'eva[12]	293	Tewari *et al.*[21]	298

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

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

where $\ln x_{\min,1} = -14.58$, $\Delta_{\mathrm{sln}} C_p / R = 53.5$, and $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 15.

All the experimental and reference data are listed in Table 16 and shown in Fig. 6. The Recommended and Tentative data are shown in Fig. 7.

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

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

Author (s)	T/K	Author (s)	T/K
Bittrich *et al.*[1]	298 and 313	McCants *et al.*[15]	311
Black *et al.*[2]	283–298	Polak and Lu[17]	273 and 298
Budantseva *et al.*[4]	293 and 313	Schatzberg[20]	298
Englin *et al.*[7]	273–323	Zel'venskii *et al.*[22]	296
Ghanem *et al.*[9]	296		

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

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

where $d_1 = -0.633$, $d_2 = -6.177$, $d_3 = -0.846$, $d_4 = -3.372$, and $T_r = T/524.2$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of heptane in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 17.

The experimental and reference solubility data for (2) in (1) are listed in Table 18 and shown in Fig. 8.

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

The experimental high pressure solubility of (1) in (2) have been investigated by Connolly[5] at constant temperatures 568 K–628 K and 17 220 kPa–70 910 kPa. There data were measured by one author only have not been critically evaluated.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[26] are independent data. The data reported by Bröllos *et al.*,[23] Gill *et al.*,[24] Milligan,[25] and Roof[27] lack sufficient information to justify evaluation.

References:

[1] H.-J. Bittrich, H. Gedan, and G. Feix, Z. Phys. Chem. (Leipzig) **260**, 1009 (1979).
[2] C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).
[3] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1941 (1948).
[4] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).
[5] *J. F. Connolly, J. Chem. Eng. Data* **11**, *13 (1966).*
[6] *R. Durand, C. R. Acad. Sci.* **226**, *409 (1948).*
[7] *B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel* **10**, *42 (1965).*
[8] *H. Fühner, Ber. Dtsch. Chem. Ges.* **57**, *510 (1924).*
[9] *N. A. Ghanem, M. Marek, and J. Exner, Int. J. Appl. Radiat. Isot.* **21**, *239 (1970).*
[10] *A. N. Guseva and E. I. Parnov, Radiokhimiya* **5**, *507 (1963).*
[11] *J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib.* **9**, *279 (1982).*
[12] *I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 1977.04.05.*
[13] *P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya* **13**, *885 (1973).*
[14] *C. McAuliffe, J. Phys. Chem.* **70**, *1267 (1966).*
[15] *J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem.* **45**, *454 (1953).*
[16] *H. D. Nelson and C. L. De Ligny, Recl. Trav. Chim. Pays-Bas Belg.* **87**, *528 (1968).*
[17] *J. Polak and B. C. Y. Lu, Can. J. Chem.* **51**, *4018 (1973).*
[18] *L. C. Price, Am. Assoc. Pet. Geol. Bull.* **60**, *213 (1976).*
[19] *E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim.* **53**, *1298 (1979).*
[20] *P. Schatzberg, J. Phys. Chem.* **67**, *776 (1963).*
[21] *Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data* **27**, *451 (1982).*
[22] *Ya. D. Zel'venskii, A. A. Efremov, and G. M. Larin, Khim. Tekhnol. Topl. Masel* **10**, *3 (1965).*
[23] *K. Bröllos, K. Peter, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem.* **74**, *682 (1970).*
[24] *S. J. Gill, N. F. Nichols, and I. Wadso, J. Chem. Thermodyn.* **8**, *445 (1976).*
[25] *L. H. Milligan, J. Phys. Chem.* **28**, *494 (1924).*
[26] *T. Krzyzanowska and J. Szeliga, Nafta (Katowice)* **12**, *413 (1978).*
[27] *G. Roof, J. Chem. Eng. Data* **15**, *301 (1970).*

TABLE 15. The data categories for solubility of heptane (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		Polak and Lu[17]	
277.5			Nelson and De Ligny[16]
286.7			Nelson and De Ligny[16]
288.2		Jonsson *et al.*[11]	
288.7			Fuehner[8]
289.2			Durand[6]
293.2		Jonsson *et al.*[11]	Budantseva *et al.*[4] Korenman and Aref'eva[12]
298.2	Krasnoshchekova and Gubergrits[13] McAuliffe[14] Rudakov and Lutsyk[19]	Jonsson *et al.*[11] Nelson and De Ligny[16] Polak and Lu[17] Price[18] Tewari *et al.*[21]	Booth and Everson[3]
303.2		Jonsson *et al.*[11]	
308.2		Jonsson *et al.*[11] Nelson and De Ligny[16]	
311.0			McCants *et al.*[15]
313.2			Budantseva *et al.*[4]
313.3		Price[18]	
318.2		Nelson and De Ligny[16]	
328.9		Price[18]	
344.7			Guseva and Parnov[10]
372.3		Price[18]	
381.2			Guseva and Parnov[10]
391.2		Price[18]	
409.8		Price[18]	
423.6		Price[18]	
454.2			Guseva and Parnov[10]
460.2			Guseva and Parnov[10]

TABLE 16. Experimental values for solubility of heptane (1) in water (2)

T/K	Experimental values x_1 (R = recommended, T = tentative, D = doubtful)	Reference values $x_1 \pm 30\%$
273.2	$7.88\cdot10^{-7}$ (T; Ref. 17)	$7.5\cdot10^{-7}$
277.5	$3.51\cdot10^{-7}$ (D; Ref. 16)	$6.8\cdot10^{-7}$
286.7	$3.63\cdot10^{-7}$ (D; Ref. 16)	$5.9\cdot10^{-7}$
288.2	$4.80\cdot10^{-7}$ (T; Ref. 11)	$5.8\cdot10^{-7}$
288.7	$9.00\cdot10^{-6}$ (D; Ref. 8)	$5.7\cdot10^{-7}$
289.2	$1.80\cdot10^{-6}$ (D; Ref. 6)	$5.7\cdot10^{-7}$
293.2	$3.00\cdot10^{-6}$ (D; Ref. 4), $4.62\cdot10^{-7}$ (T; Ref. 11), $1.10\cdot10^{-5}$ (D; Ref. 12)	$5.5\cdot10^{-7}$
298.2	$4.90\cdot10^{-5}$ (D; Ref. 3), $4.51\cdot10^{-7}$ (T; Ref. 11), $5.00\cdot10^{-7}$ (R; Ref. 13), $5.30\cdot10^{-7}$ (R; Ref. 14), $3.78\cdot10^{-7}$ (T; Ref. 16), $6.05\cdot10^{-7}$ (T; Ref. 17), $4.00\cdot10^{-7}$ (T; Ref. 18), $5.20\cdot10^{-7}$ (R; Ref. 19), $6.45\cdot10^{-7}$ (T; Ref. 21)	$5.3\cdot10^{-7}$
303.2	$4.47\cdot10^{-7}$ (T; Ref. 11)	$5.2\cdot10^{-7}$
308.2	$4.53\cdot10^{-7}$ (T; Ref. 11), $4.07\cdot10^{-7}$ (T; Ref. 16)	$5.2\cdot10^{-7}$
311.0	$2.00\cdot10^{-4}$ (D; Ref. 15)	$5.2\cdot10^{-7}$
313.2	$1.00\cdot10^{-5}$ (D; Ref. 4)	$5.3\cdot10^{-7}$
313.3	$5.00\cdot10^{-7}$ (T; Ref. 18)	$5.3\cdot10^{-7}$
318.2	$4.32\cdot10^{-7}$ (T; Ref. 16)	$5.4\cdot10^{-7}$
328.9	$5.60\cdot10^{-7}$ (T; Ref. 18)	$6.0\cdot10^{-7}$
344.7	$1.80\cdot10^{-5}$ (D; Ref. 10)	$7.5\cdot10^{-7}$
372.3	$1.01\cdot10^{-6}$ (T; Ref. 18)	$1.4\cdot10^{-6}$
381.2	$2.90\cdot10^{-5}$ (D; Ref. 10)	$1.7\cdot10^{-6}$
391.2	$2.05\cdot10^{-6}$ (T; Ref. 18)	$2.3\cdot10^{-6}$
409.8	$4.91\cdot10^{-6}$ (T; Ref. 18)	$4.1\cdot10^{-6}$
423.6	$7.86\cdot10^{-6}$ (T; Ref. 18)	$6.6\cdot10^{-6}$
454.2	$1.14\cdot10^{-4}$ (D; Ref. 10)	$2.0\cdot10^{-5}$
460.2	$1.21\cdot10^{-4}$ (D; Ref. 10)	$2.6\cdot10^{-5}$

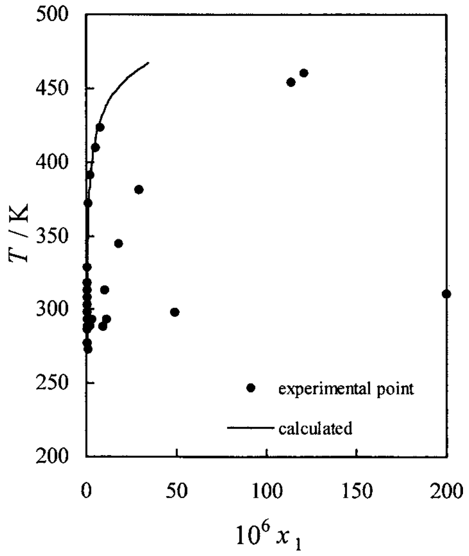

FIG. 6. All the solubility data for heptane (1) in water (2).

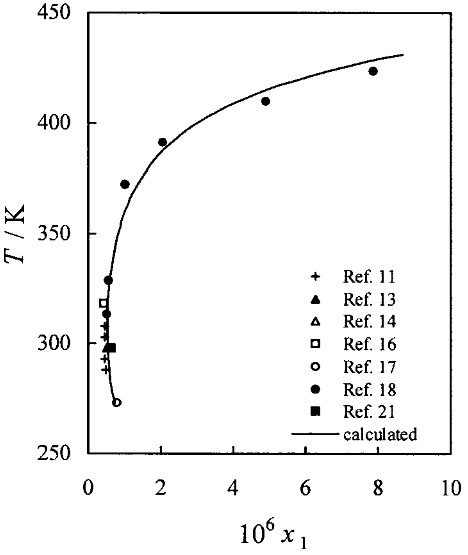

FIG. 7. Recommended and tentative solubility data for heptane (1) in water (2).

TABLE 17. The data categories for solubility of water (2) in heptane (1)

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		Englin *et al.*[7] Polak and Lu[17]	
283.2		Englin *et al.*[7]	Black *et al.*[2]
293.2		Budantseva *et al.*[4] Englin *et al.*[7]	Black *et al.*[2]
295.7			Ghanem *et al.*[9]
296.2			Zel'venskii *et al.*[22]
298.2		Bittrich *et al.*[1] Polak and Lu[17] Schatzberg[20]	Black *et al.*[2]
303.2		Englin *et al.*[7]	
311.0			McCants *et al.*[15]
313.2		Bittrich *et al.*[1]	Budantseva *et al.*[4] Englin *et al.*[7]
323.2			Englin *et al.*[7]

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

T/K	Experimental values x_2 (R=recommended, T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2	$1.50\cdot 10^{-4}$ (T; Ref. 7), $1.45\cdot 10^{-4}$ (T; Ref. 17)	$1.9\cdot 10^{-4}$
283.2	$4.28\cdot 10^{-4}$ (D; Ref. 2), $3.00\cdot 10^{-4}$ (T; Ref. 7)	$3.0\cdot 10^{-4}$
293.2	$7.56\cdot 10^{-4}$ (D; Ref. 2), $7.00\cdot 10^{-4}$ (D; Ref. 2), $5.00\cdot 10^{-4}$ (T; Ref. 4), $5.34\cdot 10^{-4}$ (T; Ref. 7)	$4.8\cdot 10^{-4}$
295.7	$3.19\cdot 10^{-4}$ (D; Ref. 9)	$5.4\cdot 10^{-4}$
296.2	$7.73\cdot 10^{-4}$ (D; Ref. 22)	$5.5\cdot 10^{-4}$
298.2	$6.70\cdot 10^{-4}$ (T; Ref. 1), $8.39\cdot 10^{-4}$ (D; Ref. 2), $4.56\cdot 10^{-4}$ (T; Ref. 17), $5.06\cdot 10^{-4}$ (T; Ref. 20)	$6.0\cdot 10^{-4}$
303.2	$9.57\cdot 10^{-4}$ (T; Ref. 7)	$7.5\cdot 10^{-4}$
311.0	$6.60\cdot 10^{-3}$ (D; Ref. 15)	$1.0\cdot 10^{-3}$
313.2	$8.70\cdot 10^{-4}$ (T; Ref. 1), $7.00\cdot 10^{-4}$ (D; Ref. 4), $1.71\cdot 10^{-3}$ (D; Ref. 7)	$1.1\cdot 10^{-3}$
323.2	$2.66\cdot 10^{-3}$ (D; Ref. 7)	$1.7\cdot 10^{-3}$

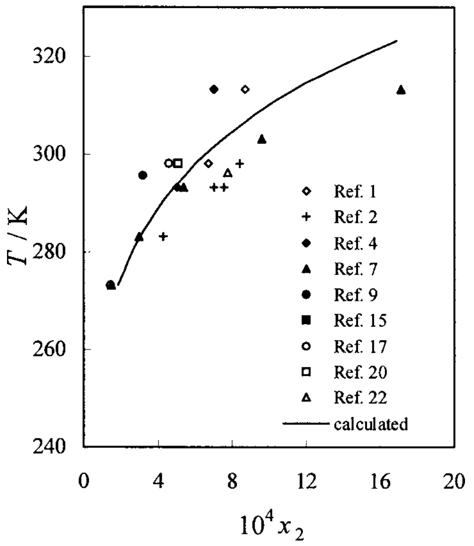

FIG. 8. All the solubility data for water (2) in heptane (1).

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	H.-J. Bittrich, H. Gedan, and G. Feix, Z. Phys. Chem. (Leipzig) **260**, 1009 (1979).
Variables:	**Prepared By:**
Temperature: 25 °C–40 °C	M. C. Haulait-Pirson

Experimental Data

Solubility of heptane in water

t/°C	x_1 (compiler)	$g(1)$/100 g sln (compiler)	mg (1)/kg (2)
Unspecified	$6.6\cdot 10^{-7}$	0.00037	3.7

Solubility of water in heptane

t/°C	x_2 (compiler)	$g(2)$/100 g sln (compiler)	mg (2)/kg (1)
25	$6.73\cdot 10^{-4}$	0.0121	121
40	$8.68\cdot 10^{-4}$	0.0156	156

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was shaken in the absence of air at a specified temperature and then thermostatted for 48 h. The equilibrated phases were sampled and analyzed by gas chromatography using a flame ionization detector. A 3 m steel column of 15% nitrile silicone on Porolith, 110 °C and a 3 m steel column of 1.5 g CaC_2 and 10% SE 30 on chromaton N, 120 °C were used for (1) and (2), respectively.

Source and Purity of Materials:

(1) Source not specified; distilled or crystallized; purity tested by gas chromatography.
(2) Not specified.

Estimated Error:

Solubility: ±9% (type of error not specified).

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).
Variables: Temperature: 10 °C–25 °C	**Prepared By:** M. C. Haulait-Pirson

Experimental Data

Solubility of water in heptane at a total saturation pressure of 1 atm

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln	$g(2)$/100 g sln (compiler)
10	4.28	0.0077	0.0077
20	7.56	0.0136	0.0136
20	7.00	0.0126	0.0126
25	8.39	0.0151	0.0151

Auxiliary Information

Method/Apparatus/Procedure:

The method described in Joris and Taylor[1] in which tritium oxide acts as a tracer, was used.
Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred to the counter through equilibration with ethanol vapor.

Source and Purity of Materials:

(1) Ohio State University under an American Petroleum Institute project; purity not specified; used as received.
(2) Not specified.

Estimated Error:

Solubility: a few percent (type of error not specified).

References:

[1] G. G. Joris and H. S. Taylor, J. Chem. Phys. **16**, 45 (1948).

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
Variables: One temperature: 25.0 °C (298.2 K)	**Prepared By:** G. T. Hefter

Experimental Data

The solubility of heptane in water at 25.0 °C was reported to be <0.04 mL(1)/100 mL(2).

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

Auxiliary Information

Method/Apparatus/Procedure:

A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.02 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath and then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute, measured directly in the tube, from the total added.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976); Deposited doc. VINITI 438-76 (1976).
Variables:	**Prepared By:**
Temperature: 20 °C and 40 °C	A. Maczynski

Experimental Data

Solubility of heptane in water

t/°C	$10^5 \cdot x_1$	$10^3 \cdot g(1)$/100 g sln (compiler)
20	0.3	2
40	1	6

Solubility of water in heptane

t/°C	$10^4 \cdot x_2$	$10^3 \cdot g(2)$/100 g sln (compiler)
20	5	9
40	7	13

Auxiliary Information

Method/Apparatus/Procedure:

Nothing specified in the paper.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).
Variables:	**Prepared By:**
Temperature: 295 °C–355 °C Pressure: 170 atm–700 atm	M. C. Haulait-Pirson

Experimental Data

Solubility of heptane in water

t/°C	x_1 (compiler)	$g(1)$/100 g sln	P/atm	P/MPa (compiler)
295	0.0020	1.1	170	17.22
295	0.0020	1.1	250	25.32
295	0.0020	1.1	500	50.65
295	0.0020	1.1	700	70.91
330	0.0061	3.3	200	20.26
330	0.0061	3.3	300	30.39
330	0.0061	3.3	500	50.65
350	0.0069	3.7	195	19.75
350	0.0107	5.7	210	21.27
350	0.0187	9.6	260	26.34
350	0.0196	10.0	280	28.36
350	0.0187	9.6	310	31.40
350	0.0156	8.1	370	37.48
350	0.0107	5.7	550	55.72
355	0.0202	10.3	230	23.30
355	0.0273	13.5	240	24.31
355	0.0417	19.5	250	25.32
355	0.0557	24.7	245	24.82
355	0.1139	41.7	320	32.42
355	0.0885	35.7	310	31.40
355	0.0693	29.3	300	30.39
355	0.0559	24.8	300	30.39
355	0.0417	19.5	305	30.90
355	0.0273	13.5	345	34.95
355	0.0202	10.3	390	39.51

Comments and Additional Data: Upper critical solution temperature: 353 °C at $P = 290$ atm (29.83 MPa).
The uncertainty in the CST is about 2 °C and that of the corresponding pressure about 10 atm.

Auxiliary Information

Method/Apparatus/Procedure:

The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.

Source and Purity of Materials:

(1) Phillips reagent grade; better than 99.8%; used as received.
(2) Distilled and deaerated.

Estimated Error:

Temperature: ±0.02 °C.
Solubility: ±2 atm (accuracy).

Components:
(1) Heptane; C_7H_{16}; [142-82-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. Durand, C. R. Hebd. Seances Acad. Sci. **226**, 409 (1948).

Variables:
One temperature: 16 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of heptane in water at 16 °C was reported to be 0.015 mL (1)/L (2).

With the assumption of a solution density of 1.00 $g\cdot$/mL and a density value of 0.6868 $g\cdot$/mL for heptane at 16 °C (Timmermans[2]), the corresponding mass percent is 0.0010 g sln and the corresponding mole fraction, x_1, is $1.8\cdot 10^{-6}$ (compiler).

Auxiliary Information

Method/Apparatus/Procedure:
The thermostatic method described in Durand[1] was used. Addition of pipetted volumes of (1)–(2) followed by shaking was repeated until appearance of turbidity.

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

Estimated Error:
Solubility: ±0.005 mL(1)/L(2).

References:
[1] R. Durand, C. R. Hebd. Seances Acad. Sci. **223**, 898 (1946).
[2] J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

Components:
(1) Heptane; C_7H_{16}; [142-82-5]
(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: 0 °C–50 °C

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

Experimental Data

Solubility of water in heptane

$t/°C$	$10^4\cdot x_2$ (compiler)	$g(2)/100$ g sln
0	1.50	0.0027
10	3.00	0.0054
20	5.34	0.0096
30	9.57	0.0172
40	17.1	0.0308
50	26.6	0.0480

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	H. Fühner, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).
Variables: One temperature: 15.5 °C	**Prepared By:** M. C. Haulait-Pirson

Experimental Data

The solubility of heptane in water at 15.5 °C was reported to be 0.007 mL (1)/100 mL sln or 0.005 $g(1)$/100 g sln.

The corresponding mole fraction, x_1, calculated by the compiler is $0.9 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a stoppered measuring cylinder pipetted volumes of weighed amounts of (1) were added with shaking to 50, 100, or 1000 mL of (2) until a completely clear solution was 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:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	N. A. Ghanem, M. Marek, and J. Exner, Int. J. Appl. Radiat. Isotop. **21**, 239 (1970).
Variables: One temperature: 22.5 °C	**Prepared By:** M. C. Haulait-Pirson

Experimental Data

The solubility of water in heptane at 22.5 °C was reported to be $3.93 \cdot 10^{-3}$ $g(2)$/100 mL(1) or $5.73 \cdot 10^{-3}$ $g(2)$/100 g(1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are $5.73 \cdot 10^{-3}$ $g(2)$/100 g sln and $3.19 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:

A volume of standardized radioactive water was injected in a vessel containing dry (1). The vessel was then closed and the contents were shaken and stirred. The vessel was then left for the excess water to settle to the bottom and sides and to ensure equilibrium. Portions of (1) saturated with (2) were added to a scintillation mixture and counted.

Source and Purity of Materials:

(1) Source not specified; purified by shaking with a mixture of H_2SO_4 and P_2O_5, kept over KOH, then distilled and the distillate refluxed over NaOH; residual water content $<5 \cdot 10^{-6}$ mol·/L.
(2) Not specified.

Estimated Error:

Temperature: ±1 °C.
Solubility: ±10% (type of error not specified).

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	A. N. Guseva and E. I. Parnov, Radiokhimiya **5**, 507 (1963).
Variables: Temperature: 71.5 °C–187 °C	**Prepared By:** A. Maczynski

Experimental Data

Solubility of heptane in water

$t/°C$	$10^5 \cdot x_1$	$g(1)/100$ g sln (compiler)
71.5	1.8	0.010
108	2.9	0.016
181	11.4	0.0633
187	12.07	0.0671

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in Khazanova.[1]

Source and Purity of Materials:

(1) Not specified.
(2) Distilled.

Estimated Error:

Not specified.

References:

[1] P. E. Khazanova, Tr. Gos. Inst. Azotn. Promyshl. **4**, 5 (1954).

Components:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. **9**, 279 (1982).
Variables: Temperature: 15 °C–35 °C	**Prepared By:** G. T. Hefter

Experimental Data

Solubility of heptane in water

$t/°C$	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot g(1)/100$ g sln (compiler)	mg (1)/kg sln
15	4.80	2.67	2.67
20	4.62	2.57	2.57
25	4.51	2.51	2.51
30	4.47	2.49	2.49
35	4.53	2.52	2.52

[a] Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinitive solution 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 absorbed in a porous polymer trap and the 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, >99.7%, used as received.
(2) Not specified.

Estimated Error:

Not specified.

References:

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

Components:

(1) Heptane; C_7H_{16} ; [142-82-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 1977.04.05.

Variables:

One temperature: 20 °C

Prepared By:

A. Maczynski

Experimental Data

The solubility of heptane in water at 20 °C was reported to be 0.06 $g(1)/L(2)$.

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.006 $g(1)/100$ g sln and $1.1 \cdot 10^{-5}$. The assumption that 1.00 L sln=1.00 kg sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

About 100–500 mL (2) was placed in a glass cylinder and 10–50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2–3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5–1.5 min.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:

(1) Heptane; C_7H_{16} ; [142-82-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski

Experimental Data

The solubility of heptane in water at 25 °C was reported to be $x_1 = 5.0 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $2.8 \cdot 10^{-4} g(1)/100$ g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and 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.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:

(1) Heptane; C_7H_{16}; [142-82-5]
(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 heptane in water at 25 °C was reported to be 2.93 mg (1)/kg sln $[0.000293\ g(1)/100\ g\ \text{sln}]$.

The corresponding mole fraction, x_1, calculated by the compiler, is $5.3\cdot 10^{-7}$. The same value is also reported in the two papers by McAulifferefs.[1,2]

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 μL sample of the (1) saturated water was withdrawn with a Hamilton syringe and injected into the fractionator of 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: 0.20 mg (1)/kg sln (standard deviation of mean).

References:

[1] C. McAuliffe, Nature (London) **200**, 1092 (1963).
[2] C. McAuliffe, Am. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

Components:

(1) Heptane; C_7H_{16}; [142-82-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454 (1953).

Variables:

One temperature: 100 °F (311 K)

Prepared By:

G. T. Hefter

Experimental Data

The solubility of heptane in water at 100 °F (311 K) was reported to be $<0.1\ g(1)/100\ g\ \text{sln}$. The corresponding mole fraction, x_1, calculated by the compiler, is $<2\cdot 10^{-4}$.

The solubility of water in heptane at 100 °F (311 K) was reported to be $0.12\ g(2)/100\ g\ \text{sln}$. The corresponding mole fraction, x_2, calculated by the compiler, is $6.6\cdot 10^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:

The method was essentially that of Washburn *et al.*[1] and involved titration of the second component to the cloud point, in a constant temperature bath.

Source and Purity of Materials:

(1) Phillips; pure grade; used without further purification; n_D^{20} 1.3974.
(2) Distilled.

Estimated Error:

Not specified.

References:

[1] E. R. Washburn, V. Hnizda, and R. D. Vold, J. Am. Chem. Soc. **53**, 3232 (1931).

Components:
(1) Heptane; C_7H_{16} ; [142-82-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. D. Nelson and C. L. De Ligny, Recl. Trav. Chim. Pays-Bas Belg. **87**, 528 (1968).

Variables:
Temperature: 4.3 °C–45 °C

Prepared By:
M C. Haulait-Pirson

Experimental Data

Solubility of heptane in water

t/°C	$10^7 \cdot x_1$	mg (1)/kg sln (compiler)
4.3	3.51±0.26	1.95
13.5	3.63±0.51	2.02
25.0	4.78±0.74	2.66
35.0	4.07±0.95	2.27
45.0	4.32±1.06	2.41

Auxiliary Information

Method/Apparatus/Procedure:
The saturation vessel is drawn in the original paper. (2) was saturated with (1) via the vapor phase: a few drops of (1) were put on the bottom of a tight-fitting flask containing a small flask filled with water. Complete saturation was reached by shaking overnight in an upright position. Samples were taken from the aqueous solution with a microsyringe through a septum and injected into a gas chromatograph equipped with a flame ionization detector. The gas chromatographic conditions are described in the paper.

Source and Purity of Materials:
(1) Phillips pure grade.
(2) Tap water was refluxed for 8 h in the presence of $KMnO_4$ and KOH and distilled. The whole process was repeated once more.

Estimated Error:
Solubility: error given above (90% probability interval).

Components:
(1) Heptane; C_7H_{16} ; [142-82-5]
(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 heptane in water

t/°C	$10^7 \cdot x_1$ (compiler)	mg (1)/kg sln
0^a	7.9	4.39^c
25^b	6.1	3.37^c

Solubility of water in heptane

t/°C	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0^a	1.45	26^d
25^b	4.56	82^e

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

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:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
Temperature: 25 °C–150.4 °C	F. Kapuku

Experimental Data

Solubility of heptane in water at system pressure

t/°C	10^7x_1 (compiler)	$g(1)$/100 g sln (compiler)	mg (1)/kg (2)
25.0	4.0	0.000224	2.24±0.04
40.1	4.7	0.000263	2.63±0.05
55.7	5.6	0.000311	3.11±0.11
99.1	10.1	0.000560	5.60±0.17
118.0	20.5	0.00114	11.4±0.4
136.6	49.1	0.00273	27.3±0.9
150.4	78.6	0.00437	43.7±1.0

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 oven of a gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample was then transferred to a 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:	**Original Measurements:**
(1) Heptane; C_7H_{16} ; [142-82-5] (2) Water; H_2O; [7732-18-5]	E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Data

The authors reported the partition coefficient α of heptane between the gas and aqueous phase. $\alpha = 84 \pm 4$. $\alpha = C_g / C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25 °C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of P (where P is the vapor pressure in mm of Hg) is taken from Ref. 1. $P = 45.81$ mm of Hg and $\log C_g = \log P - 4.269 = -2.61$ expressed in moles per liter. Therefore $C_s = 2.9 \cdot 10^{-5}$ moles/L.

With the assumption of a solution density of 1.00 g·/mL, the corresponding mass percent is 0.00029 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $5.2 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium distribution was attained after shaking a thermostatted reactor for 10 min containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.

Source and Purity of Materials:

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

Estimated Error:

Solubility: ±10% (estimated by the compiler).

References:

[1] J. Hine and P. K. Mooker, Org. Chem. **4**, 292 (1975).

Components:

(1) Heptane; C_7H_{16} ; [142-82-5]
(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 heptane at 25 °C was reported to be 91 mg (2)/kg sln corresponding to a mole fraction, x_2 , of $5.06 \cdot 10^{-4}$ and to a mass percent of 0.0091 $g(1)$/100 g sln.

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 a 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) Eastman Organic Chemicals; doubly distilled; 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% (deviation from the mean).

Components:

(1) Heptane; C_7H_{16} ; [142-82-5]
(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 heptane in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$3.57 \cdot 10^{-5}$	$3.59 \cdot 10^{-4}$	$6.45 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used, 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 thermosttated 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. De Voe, 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:	Original Measurements:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Ya. D. Zel'venskii, A. A. Efremov, and G. M. Larin, Khim. Tekhnol. Topl. Masel **10**, 3 (1965).
Variables:	**Prepared By:**
One temperature: 23 °C	A. Maczynski

Experimental Data

The solubility of water in heptane at 23 °C was reported to be 0.0139 $g(2)/100$ g sln.

The corresponding mole fraction solubility, x_2, $7.73\cdot 10^{-4}$, was calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions of tritium labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through the vessel with (2) and next through the vessel (1) and frozen. In the second, about 500 mL of (1) and 1 mL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.

Source and Purity of Materials:

(1) Source not specified; pure grade; shaken with concentration H_2SO_4; washed with water, dried over sodium, and distilled; purity not specified; b.p. 98.43 °C, m.p. −90.8 °C.

(2) Source not specified; commercial; 1 Ci/mL HTO; used as received.

Estimated Error:

Not specified.

2.20. Heptane+Heavy Water

Components:	Original Measurements:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Deuterium oxide (heavy water); D_2O; [7789-20-0]	A. N. Guseva and E. I. Parnov, Radiokhimiya **5**, 507 (1963).
Variables:	**Prepared By:**
Temperature: 68 °C–193 °C	A. Maczynski

Experimental Data

Solubility of heptane in deuterium oxide

$t/°C$	$10^5\cdot x_1$	$g(1)/100$ g sln (compiler)
68	1.51	0.0076
109	2.8	0.0140
158	6.24	0.0312
193	14.9	0.0745

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in Khazanova.[1]

Source and Purity of Materials:

(1) Not specified.

(2) Distilled.

Estimated Error:

Not specified.

References:

[1] P. E. Khazanova, Tr. Gos. Inst. Azotn. Promyshl. **4**, 5 (1954).

2.21. 2-Methylhexane+Water

Components:	**Original Measurements:**
(1) 2-Methylhexane; C_7H_{16} ; [591-76-4] (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-methylhexane

$t/°C$	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.12	0.0056
20	5.73	0.0103
30	10.12	0.0182

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 evolved hydrogen volume was measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:

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

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) 2-Methylhexane; C_7H_{16} ; [591-76-4] (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 2-methylhexane in water at 25 °C and at system pressure was reported to be 2.54 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $2.54 \cdot 10^{-4} g(1)$/100 g sln and $4.57 \cdot 10^{-7}$.

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: ±0.02 mg(1)/kg(2).

2.22. 3-Methylhexane+Water

Components:	**Evaluators:**
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, August, 2003.

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

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

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

where $\ln x_{\min,1} = -14.21$, $\Delta_{\text{sln}} C_p / R = 51.6$, 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 19. The data of Polak and Lu[1] are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Price[2] are in poor agreement with the reference data and are Doubtful.

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

The experimental solubility data 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:

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

where $d_1 = -0.789$, $d_2 = -6.140$, $d_3 = -0.530$, $d_4 = -3.835$, and $T_r = T/520.6$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of 3-methylhexane 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 20. The data of Polak and Lu[1] at 273 K, are in good agreement with the reference data and are Tentative. The remaining data at 298 K are in poor agreement with the reference data and are Doubtful.

Rejected and Inaccessible Data

In the opinion of the evaluators, uncertainty exists as to whether the solubility measurements reported by Krzyanowski and Szeliga[3] are independent data.

References:

[1] J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[2] L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[3] T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

TABLE 19. Experimental values for solubility of 3-methylhexane (1) in water (2)

T/K	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$9.41 \cdot 10^{-7}$ (T; Ref. 1)	$1.1 \cdot 10^{-6}$
298.2	$8.89 \cdot 10^{-7}$ (T; Ref. 1) $4.70 \cdot 10^{-7}$ (D; Ref. 2)	$7.7 \cdot 10^{-7}$

TABLE 20. Experimental values for solubility of water (2) in 3-methylhexane (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2	$1.39 \cdot 10^{-4}$ (T; Ref. 1)	$1.9 \cdot 10^{-4}$
298.2	$4.12 \cdot 10^{-4}$ (D; Ref. 1)	$6.1 \cdot 10^{-4}$

Components:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4]
(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 3-methylhexane in water

$t/°C$	$10^7 \cdot x_1$ (compiler)	mg (1)/kg sln
0^a	9.41	5.24^c
25^b	8.89	4.95^c

Solubility of water in 3-methylhexane

$t/°C$	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0^a	1.39	25^d
25^b	4.12	74^e

[a–e]See Estimated Error

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by the Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

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) ±1.7%; (d) ±4.7%; (e) ±3.1% (mean).

Components:
(1) 3-methylhexane; C_7H_{16}; [589-34-4]
(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 3-methylhexane in water at 25 °C and at system pressure was reported to be 2.64 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $2.64 \cdot 10^{-4} g(1)/100$ g sln and $4.75 \cdot 10^{-7}$.

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: ±0.08 mg(1)/kg(2).

2.23. 2,2,3-Trimethylbutane+Water

Components:	**Original Measurements:**
(1) 2,2,3-Trimethylbutane; C_7H_{16} ; [464-06-2] (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: 0 °C–50 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Data

Solubility of water in 2,2,3-trimethylbutane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
0	1.50	0.0027
10	3.17	0.0057
20	8.90	0.0106
30	10.23	0.0184
40	17.51	0.0315
50	28.15	0.0507

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Not specified.

3. System Index

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

4. Registry Number Index

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

5. Author Index

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

IUPAC-NIST SOLUBILITY DATA SERIES