IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater Revised and Updated. Part 7. C_8H_{12}–C_8H_{18} Hydrocarbons with Water

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The mutual solubility and related liquid-liquid equilibria of C_8H_{12}–C_8H_{18} hydrocarbons with water are exhaustively and critically reviewed. Reports of experimental determinations of solubility in 20 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For 5 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. © *2005 American Institute of Physics.*

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Key words: C_8H_{12}–C_8H_{18} hydrocarbons; critical evaluation; liquid-liquid equilibria; solubilities; water.

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1. Preface

1.1. Scope of This Volume

This paper is Part 7 of a revised and updated version of an earlier compilation and evaluation of the mutual solubility of water and hydrocarbon compounds containing five or more carbon atoms (Shaw[1,2]). This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

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

Detailed introductory material including explanations of the formats of compilation and evaluation, definitions of commonly used measures of solubility, and the scope of the Solubility Data Series can be found in Part 1 (Maczynski and Shaw[6]). The derivation of the smoothing equations used to calculate reference values can be found in Parts 1 and 2 (Maczynski and Shaw[6,7]) and in Wisniewska-Goclowska *et al.*[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-Alkaline Water Systems*, J. Phys. Chem. Ref. Data **33**, 549 (2004).

[5] M. Goral, A. Maczynski, and B. Wisniewska-Goclowska, *Recommended Liquid-Liquid Equilibrium Data. Part. 2. Unsaturated Hydrocarbon-Water Systems*, J. Phys. Chem. Ref. Data **33**, 579 (2004).

[6] 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).

[7] 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).

[8] B. Wisniewska-Goclowska, M. Goral, and A. Maczynski, *Recommended Liquid-Liquid Equilibrium Data. Part 3. Alkylbenzene-Water Systems*, J. Phys. Chem. Ref. Data **33**, 1159 (2004).

2. C_8H_{12}–C_8H_{18} Hydrocarbons with Water

2.1. 4-Vinyl-1-cyclohexene+Water

Components:

(1) 4-Vinyl-1-cyclohexene; C_8H_{12} ; [100-40-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

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

Experimental Values

The solubility of 4-vinyl-1-cyclohexene in water at 25 °C was reported to be 50 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.005 g (1)/100 g sln and $8.3 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

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

2.2. 1-Propenylcyclopentane+Water

Components:

(1) 1-Propenylcyclopentane; C_8H_{14} ; [5623-78-9]
(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:

One temperature: 30 °C

Prepared By:

A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in 1-propenylcyclopentane at 30 °C was reported to be 0.0383 $g(2)$/100 g sln.

The corresponding value mole fraction, x_2 , calculated by the compilers is $2.34 \cdot 10^{-3}$.

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.

2.3. 1,7-Octadiene+Water

Components:	**Original Measurements:**
(1) 1,7-Octadiene; C_8H_{14}; [3710-30-3] (2) Water; H_2O; [7732-18-5]	A. O. Emelyanov, L. V. Melnik, and B. N. Bobylev, Zh. Prikl. Khim. (Leningrad) **64**, 1700 (1991).
Variables:	**Prepared By:**
Temperature: 293.15 and 360.15 K	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1,7-octadiene in water

T/K	$g(1)$/100 g sln (compilers)	x_1
293.15	0.18	0.0003
360.15	8.47	0.0149

Solubility of water in 1,7-octadiene

T/K	$g(2)$/100 g sln (compilers)	x_2
293.15	0.0033	0.0002
360.15	0.0082	0.0005

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. No details were reported in the paper.

Source and Purity of Materials:

(1) Prepared in own laboratory; distilled; purity >99.5 mass %.
(2) Twice distilled.

Estimated Error:

Not stated.

2.4. 1-Octyne+Water

Components:	**Original Measurements:**
(1) 1-Octyne; C_8H_{14}; [629-05-0] (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 Values

The solubility of 1-octyne in water at 25 °C was reported to be 24 mg (1)/kg (2).
The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0024 $g(1)$/100 g sln and $4.4 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 0.8 mg (1)/kg (2) (std. dev. of mean)

2.5. Cyclooctane+Water

Components:
(1) Cyclooctane; C_8H_{16}; [292-64-8]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of cyclooctane in water at 25 °C was reported to be 7.9 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is $1.27 \cdot 10^{-6}$. 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 mL 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: 1.8 mg (1)/kg sln (std. dev. from mean).

References:

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

2.6. cis-1,2-Dimethylcyclohexane+Water

Components:
(1) *cis*-1,2-Dimethylcyclohexane; C_8H_{16}; [2207-01-4]
(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 Values

The solubility of *cis*-1,2-dimethylcyclohexane in water at 25 °C was reported to be 6.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00060 $g(1)$/100 g sln and $9.6 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

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

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

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 0.8 mg (1)/kg (2) (std. dev. of mean).

2.7. 1,4-Dimethylcyclohexane+Water

Components:	**Original Measurements:**
(1) 1,4-Dimethylcyclohexane; C_8H_{16}; [589-90-2] (2) Water; H_2O; [7732-18-5]	A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).
Variables:	**Prepared By:**
Temperature: 57 °C–240 °C	M. C. Haulait-Pirson

Experimental Values

1,4-dimethylcyclohexane in water

t/°C	$10^4 \cdot x_1$	$g(1)/100$ g sln
57	0.027	0.0017
105	0.090	0.0056
165	0.422	0.0263
240	4.120	0.257

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Not specified.

References:

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

2.8. trans-1,4-Dimethylcyclohexane+Water

Components:	**Original Measurements:**
(1) *trans*-1,4-Dimethylcyclohexane; C_8H_{16}; [2207-04-7] (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 Values

The solubility of *trans*-1,4-dimethylcyclohexane in water at 25 °C and at system pressure was reported to be 3.84 mg (1)/kg (2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are $3.84 \cdot 10^{-4}$ $g(1)/100$ g sln and $6.16 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±1 °C.
Solubility: ±0.17 mg(1)/kg(2).

2.9. Ethylcyclohexane+Water

Components:	**Evaluators:**
(1) Ethylcyclohexane; C_8H_{16}; [1678-91-7] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

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

The experimental solubility data for (1) in (2) have been investigated by Guseva and Parnov[1] at 352–486 K and Heidman *et al.*[2] at 311–561 K at pressures to 8830 kPa.

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

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

where $\ln x_{\mathrm{min},1} = -14.18$, $\Delta_{\mathrm{sln}} C_p / R = 51.5$, 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 1 and shown in Fig. 1. The data of Heidman *et al.*[2] at 367 K and 479–553 K are in good agreement (within 30% relative standard deviation) with the reference date and are Tentative. The data of Guseva and Parnov[1] and Heidman *et al.*[2] at 311 K and 423 K 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 Ethylcyclohexane (1)

The experimental solubility data for (2) in (1) have been investigated by Heidman *et al.*[2] at 311–561 K and 10–9930 kPa.

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 $d_1 = -0.006$, $d_2 = -5.839$, $d_3 = -1.937$, $d_4 = -2.037$, and $T_r = T/563.2$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of ethylcyclohexane 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 2 and shown in Fig. 2. Since only one experimental data point is available at each temperature, no data can be Recommended. The data of Heidman *et al.*[2] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:

[1] A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. Khim. **19**, 77 (1964).
[2] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

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

T/K	P/kPa	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
311.5		$1.10\cdot10^{-6}$ (D; Ref. 2)	$8.1\cdot10^{-7}$
352.2		$7.70\cdot10^{-6}$ (D; Ref. 1)	$1.5\cdot10^{-6}$
367.6	117	$2.40\cdot10^{-6}$ (T; Ref. 2)	$2.2\cdot10^{-6}$
415.7		$6.39\cdot10^{-5}$ (D; Ref. 1)	$1.0\cdot10^{-5}$
423.4	647	$2.00\cdot10^{-5}$ (D; Ref. 2)	$1.3\cdot10^{-5}$
449.2		$2.22\cdot10^{-4}$ (D; Ref. 1)	$3.4\cdot10^{-5}$
479.5	2360	$1.21\cdot10^{-4}$ (T; Ref. 2)	$1.2\cdot10^{-4}$
486.2		$9.96\cdot10^{-4}$ (D; Ref. 1)	$1.5\cdot10^{-4}$
536.1	6690	$1.18\cdot10^{-3}$ (T; Ref. 2)	$1.2\cdot10^{-3}$
552.8	8830	$2.37\cdot10^{-3}$ (T; Ref. 2)	$2.5\cdot10^{-3}$

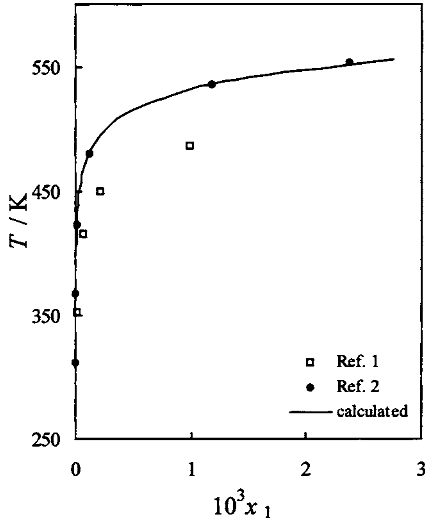

FIG. 1. All the solubility data for ethylcyclohexane (1) in water (2).

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

T/K	P/kPa	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
310.9	9.9	$8.10\cdot10^{-4}$ (T; Ref. 2)	$7.9\cdot10^{-4}$
367.6	117	$6.50\cdot10^{-3}$ (T; Ref. 2)	$5.6\cdot10^{-3}$
423.4	647	$3.00\cdot10^{-2}$ (T; Ref. 2)	$2.6\cdot10^{-2}$
479.5	2360	$1.07\cdot10^{-1}$ (T; Ref. 2)	$9.5\cdot10^{-2}$
536.1	6690	$2.90\cdot10^{-1}$ (T; Ref. 2)	$3.3\cdot10^{-1}$
552.8	8830	$4.14\cdot10^{-1}$ (T; Ref. 2)	$5.1\cdot10^{-1}$
561.4[a]	9930	$6.03\cdot10^{-1}$ (T; Ref. 2)	

[a] UCST.

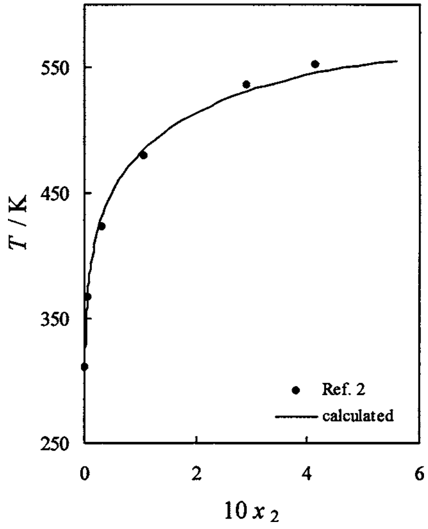

FIG. 2. All the solubility data for water (2) in ethylcyclohexane (1).

Components:	**Original Measurements:**
(1) Ethylcyclohexane; C_8H_{16} ; [1678-91-7] (2) Water; H_2O; [7732-18-5]	A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).
Variables:	**Prepared By:**
Temperature: 79–213 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of ethylcyclohexane in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g(2)	$g(1)$/100 g sln (compiler)
79	0.077	0.0048	0.0048
142.5	0.639	0.0398	0.0398
176	2.22	0.138	0.138
213	9.96	0.66	0.62

Auxiliary Information

Method/Apparatus/Procedure:

Presumably the measurements were made in sealed glass tubes, as reported in Guseva and Parnov.[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, Zh. Fiz. Khim. **37**, 2763 (1963).

Components:
(1) Ethylcyclohexane; C_8H_{16}; [1678-91-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

Variables:
Temperature: 311–561 K
Pressure: 0.01–9.9 MPa

Prepared By:
G. T. Hefter

Experimental Values

Solubility of ethylcyclohexane in water

T/K	$10^4 \cdot x_1$	$10^2 \cdot g(1)$/100 g sln (compiler)	P/MPa
311.5	0.011	0.068	not specified
367.6	0.024	0.15	0.117
423.4	0.20	1.2	0.647
479.5	1.21	7.5	2.36
536.1	11.8	73	6.69
552.8	23.7	146	8.83

Solubility of water in ethylcyclohexane

T/K	$10^2 \cdot x_2$	$g(2)$/100 g sln (compiler)	P/MPa
310.9	0.081	0.0130	0.0099[a]
367.6	0.65	0.104	0.117
423.4	3.0	0.48	0.647
479.5	10.7	1.89	2.36
536.1	29.0	6.15	6.69
552.8	41.4	10.2	8.83
561.4[b]	60.3[b]	19.6	9.93[b]

[a] Estimated by the authors from pure component data.
[b] Three phase critical point.

The three phase critical point was reported to be 561.4±0.6 K, 9.93±0.04 MPa, and $x_1 = 3.35 \cdot 10^{-3}$[1.05 $g(1)$/100 g sln, compiler].

The authors also report an equation which fits their own and related literature data over the range 273–561 K, viz.

$$\ln x_1 = -334.2468 + 14105.21/T + 47.93102 \ln T$$

$$\ln x_2 = -0.50980 - 7.4603(T_r^{-1} - 1) - 0.67885(1 - T_r)^{1/3} + 0.44796(1 - T_r)$$

where $T_r = T/561.4$

Auxiliary Information

Method/Apparatus/Procedure:

Experimental procedure was similar to that used in Tsonopoulos and Wilson.[1] Hydrocarbons were determined by gas chromatography and water by the Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.

Source and Purity of Materials:

(1) Aldrich 99+mol %; water free purity ⩾99.9 mol %, checked by gas chromatography.
(2) Distilled; no details given.

Estimated Error:

Temperature: not stated.
Solubility: 5%, relative precision of replicate analyses.
Pressure: ±1%; type of error not stated.

References:

[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).

2.10. Isopropylcyclopentane+Water

Components:
(1) Isopropylcyclopentane C_8H_{16}; [3875-51-2]
(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: 10–30 °C

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

Experimental Values

Solubility of water in isopropylcyclopentane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.68	0.0059
20	6.35	0.0102
30	9.90	0.0159

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Not specified.

2.11. 1-Octene+Water

Components:	**Evaluators:**
(1) 1-Octene; C_8H_{16} ; [111-66-0] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

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

The experimental solubility data for (1) in (2) have been investigated by Economou *et al.*[1] at 311–549 K, McAuliffe,[2] Natarajan and Venkatachalam,[3] 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:

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

where $\ln x_{1,\min} = -14.59$, $\Delta_{\mathrm{sln}} C_p/R = 59.8$, $T_{\min} = 306$ 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 Economou *et al.*,[1] McAuliffe,[2] Natarajan and Venkatachalam,[3] and Tewari *et al.*[4] are listed in Table 3 and shown in Fig. 3. The data of McAuliffe[2] at 298 K and Economou *et al.*[1] at 311 K and 478 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

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

T/K	P/kPa	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
298.2		$4.00 \cdot 10^{-7}$ (T; Ref. 2), $3.63 \cdot 10^{-6}$ (D; Ref. 3), $6.60 \cdot 10^{-7}$ (D; Ref. 4)	$4.7 \cdot 10^{-7}$
310.9		$5.0 \cdot 10^{-7}$ (T; Ref. 1)	$4.7 \cdot 10^{-7}$
366.5	124 (Ref. 1)	$1.80 \cdot 10^{-6}$ (D; Ref. 1)	$1.2 \cdot 10^{-6}$
422.0	662 (Ref. 1)	$1.40 \cdot 10^{-5}$ (D; Ref. 1)	$7.5 \cdot 10^{-6}$
477.6	2423 (Ref. 1)	$9.10 \cdot 10^{-5}$ (T; Ref. 1)	$7.9 \cdot 10^{-5}$
533.2	6840 (Ref. 1)	$6.20 \cdot 10^{-4}$ (D; Ref. 1)	$1.0 \cdot 10^{-3}$
549.8	9260 (Ref. 1)	$9.80 \cdot 10^{-4}$ (D; Ref. 1)	$2.3 \cdot 10^{-3}$

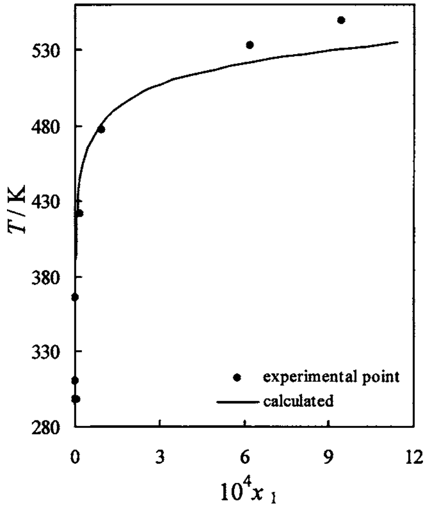

FIG. 3. All the solubility data for 1-octene (1) in water (2).

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

The experimental solubility data for (2) in (1) have been investigated by Economou *et al.*[2] at 311–549 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 $d_1 = -0.256$, $d_2 = -3.091$, $d_3 = 0.082$, $d_4 = -8.020$, and $T_r = T/550.8$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1-octene 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 4. All the data are shown in Fig. 4. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:

[1] I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
[2] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[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 4. Experimental values for solubility of water (2) in 1-octene (1)

T/K	P/kPa	Experimental values x_1 (T=tentative)	Reference values $x_2 \pm 30\%$
310.9		$1.68 \cdot 10^{-3}$ (T; Ref. 1)	$2.3 \cdot 10^{-3}$
366.5	124 (Ref. 1)	$8.70 \cdot 10^{-3}$ (T; Ref. 1)	$1.2 \cdot 10^{-2}$
422.0	662 (Ref. 1)	$4.51 \cdot 10^{-2}$ (T; Ref. 1)	$4.9 \cdot 10^{-2}$
477.6	2423 (Ref. 1)	$1.56 \cdot 10^{-1}$ (T; Ref. 1)	$1.7 \cdot 10^{-1}$
533.2	6840 (Ref. 1)	$4.19 \cdot 10^{-1}$ (T; Ref. 1)	$5.5 \cdot 10^{-1}$
549.8	9260 (Ref. 1)	$5.38 \cdot 10^{-1}$ (T; Ref. 1)	$7.7 \cdot 10^{-1}$

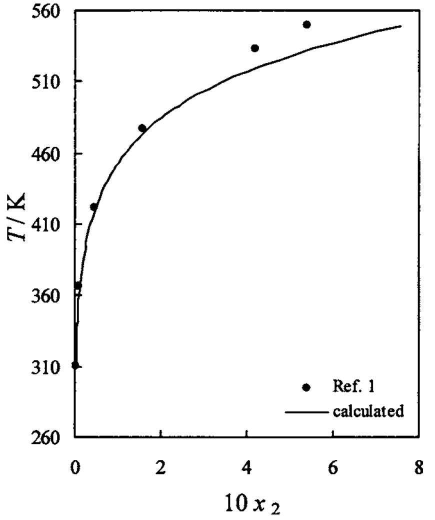

FIG. 4. All the solubility data for water (2) in 1-octene (1).

Components:

(1) 1-Octene; C_8H_{16}; [111-66-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 310.93–549.82 K
Pressure: 0.124–9.260 MPa

Prepared By:

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

Experimental Values

Solubility of 1-octene in water

T/K	P/MPa	$g(1)$/100 g sln (compilers)	$10^4 \cdot x_1$
310.93	—	0.000311	0.0050
366.48	0.124	0.00112	0.018
422.04	0.662	0.0087	0.14
477.59	2.423	0.0567	0.91
533.15	6.840	0.385	6.2
549.82[a]	9.260	0.607	9.8

Solubility of water in 1-octene

T/K	P/MPa	$g(2)$/100 g sln (compilers)	x_2
310.93	—	0.0270	0.00168
366.48	0.124	0.1407	0.00870
422.04	0.662	0.752	0.0451
477.59	2.423	2.88	0.156
533.15	6.840	10.38	0.419
539.21[b]	7.467	14.67	0.517
549.82[a]	9.260	15.75	0.538

[a] Above three-phase critical end point.

[b] Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

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

References:

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

Components:

(1) 1-Octene; C_8H_{16}; [111-66-0]
(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 Values

The solubility of 1-octene in water at 25 °C was reported to be 2.7 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are $2.7 \cdot 10^{-4}$ $g(1)$/100 g sln and $4 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 0.2 mg (1)/kg (2) (std. dev. of mean).

Components:
(1) 1-Octene; C_8H_{16}; [111-66-0]
(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 Values

The solubility of 1-octene in water was reported to be $1.979 \cdot 10^{-4}$ mol(1)/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, 0.00222 $g(1)$/100 g sln and $3.63 \cdot 10^{-6}$.

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 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: not specified.

Components:
(1) 1-Octene; C_8H_{16}; [111-66-0]
(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 Values

Solubility of 1-octene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$3.65 \cdot 10^{-5}$	$4.11 \cdot 10^{-4}$	$6.60 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used as described in deVoe *et al.*[1] and May *et al.*[2] A column was coated with an organic liquid 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 thermostatted 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).

2.12. 2-Octene+Water

Components:
(1) 2-Octene; C_8H_{16}; [111-67-1]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 15–25 °C

Prepared By:
M. C. Haulait-Pirson and G. T. Hefter

Experimental Values

Solubility of 2-octene 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/L sln[a]
15	5.3	3.3	2.92±0.14 (a)
20	4.5	2.8	2.51±0.16 (a)
25	3.9	2.4	2.16±0.15 (a)

[a] Uncertainties stated to be ''standard deviations from means.''

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

Compiler's Note: Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause (1) 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) Prepared by dehydration of 2-octanol and then washed, dried, and fractionated. Purity (no specification) was determined by chromatography.
(2) Not specified.

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

2.13. Propylcyclopentane+Water

Components:
(1) Propylcyclopentane; C_8H_{16}; [2040-96-2]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of propylcyclopentane in water at 25 °C and at system pressure was reported to be 2.04 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $2.04 \cdot 10^{-4}$ $g(1)/100$ g sln and $3.27 \cdot 10^{-7}$.

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: ±0.10 mg(1)/kg(2).

2.14. 1,1,3-Trimethylcyclopentane+Water

Components:
(1) 1,1,3-Trimethylcyclopentane; C_8H_{16} ; [4516-69-2]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 1,1,3-trimethylcyclopentane in water at 25 °C and at system pressure was reported to be 3.73 mg (1)/kg (2). The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are $3.73 \cdot 10^{-4}$ $g(1)$/100 g sln and $5.99 \cdot 10^{-7}$.

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: ±0.17 mg(1)/kg(2).

2.15. 2,3-Dimethylhexane+Water

Components:
(1) 2,3-Dimethylhexane; C_8H_{18} ; [584-94-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. G. Baker, Geochim. Cosmochim. Acta **19**, 309 (1960).

Variables:
One temperature: not specified

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 2,3-dimethylhexane in water was reported to be 0.0002 mL (1)/L (2).

Auxiliary Information

Method/Apparatus/Procedure:

The procedure is described in Baker.[1]

Source and Purity of Materials:

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

Estimated Error:
Not specified.

References:

[1] E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Preprints C61 **4**, 3 (1958).

2.16. 2,4-Dimethylhexane+Water

Components:
(1) 2,4-Dimethylhexane; C_8H_{18}; [589-43-5]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 10–30 °C

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

Experimental Values

Solubility of water in 2,4-dimethylhexane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.36	0.0053
20	6.21	0.0098
30	11.41	0.0180

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.

2.17. 3-Methylheptane+Water

Components:
(1) 3-Methylheptane; C_8H_{18}; [589-81-1]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 3-methylheptane in water at 25 °C and at system pressure was reported to be 0.792 mg (1)/kg (2).
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $7.92 \cdot 10^{-5}$ $g(1)$/100 g sln and $1.25 \cdot 10^{-7}$.

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: ±0.028 mg(1)/kg(2).

2.18. Octane+Water

Components:	Evaluators:
(1) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

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

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

Author (s)	T/K	Author (s)	T/K
Baker[1]	298	McAuliffe[9]	298
Budantseva *et al.*[3]	293	Miller and Hawthorne[10]	298–473 K (6500 kPa)
Führer[5]	289	Nelson and De Ligny[11]	278–310
Heidman[6]	311–553 (10–8860 kPa)	Polak and Lu[12]	273 and 298
Jonsson *et al.*[7]	288–308	Price[13]	298–423
Krasnoshchekova and Gubergrits[8]	298	Tewari *et al.*[15]	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:

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

where $\ln x_{\min,1} = -16.24$, $\Delta_{\mathrm{sln}} C_{\mathrm{p}}/R = 62.0$, and $T_{\min} = 306$.

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

All the experimental and reference data are listed in Table 6 and shown in Fig. 5. The Recommended and Tentative data are shown in Fig. 6.

Critical Evaluation of the Solubility of Water (2) in Octane (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
Black *et al.*[2]	293	Heidman[6]	311–553 (10–8860 kPa)
Budantseva *et al.*[3]	293	Polak and Lu[12]	273 and 298
Englin *et al.*[4]	283–303		

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:

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

where $d_1 = -0.456$, $d_2 = -5.460$, $d_3 = -0.260$, $d_4 = -4.467$, and $T_{\mathrm{r}} = T/553.8$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of octane 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 7.

The experimental and reference solubility data for (2) in (1) are listed in Table 8 and shown in Fig. 7.

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

The experimental high pressure solubility of (1) in (2) investigated by Skripka[14] at 498–538 K, and 3500 and 78 500 kPa have not been critically evaluated because only a single data set is available and because the developed method is not applied for such data.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[18] are independent data. The data reported by Roof,[16] and Scott and van Konynenburg,[17] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1] E. G. Baker, Geochim. Cosmochim. Acta **19**, 309 (1960).
[2] C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).
[3] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).
[4] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[5] H. Führer, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).
[6] J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).
[7] J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. **9**, 279 (1982).
[8] P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).
[9] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[10] D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).
[11] H. D. Nelson and C. L. De Ligny, Recl. Trav. Chim. Pays-Bas Belg. **87**, 528 (1968).
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[17] R. L. Scott and P. H. van Konynenburg, Phil. Trans. Roy. Soc., London Ser. A **298**, 495 (1980).
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TABLE 5. The data categories for solubility of octane (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[12]
278.2			Nelson and De Ligny[11]
288.2	Jonsson *et al.*[7] Nelson and De Ligny[11]		
289.2			Fuehner[5]
293.2		Jonsson *et al.*[7]	Budantseva *et al.*[3]
298.0			Miller and Hawthorne[10]
298.2	Krasnoshchekova and Gubergrits[8] McAuliffe[9]	Jonsson *et al.*[7]	Baker[1] Polak and Lu[12] Price[13] Tewari *et al.*[15]
303.2		Jonsson *et al.*[7]	
308.2		Jonsson *et al.*[7]	
310.9		Heidman[6]	
313.3		Price[13]	
318.2			Nelson and De Ligny[11]
323.0			Miller and Hawthorne[10]
342.9		Price[13]	
366.5			Heidman[6]
372.3			Price[13]
373.0			Miller and Hawthorne[10]
394.5		Price[13]	
409.8		Price[13]	
422.0			Heidman[6]
422.7		Price[13]	
423.0			Miller and Hawthorne[10]
473.0			Miller and Hawthorne[10]
479.5			Heidman[6]
536.1		Heidman[6]	
552.8		Heidman[6]	

TABLE 6. Experimental values for solubility of octane (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		$2.13\cdot 10^{-7}$ (D; Ref. 12)	$1.5\cdot 10^{-7}$
278.2		$2.60\cdot 10^{-7}$ (D; Ref. 11)	$1.4\cdot 10^{-7}$
288.2		$1.03\cdot 10^{-7}$ (R; Ref. 7), $1.40\cdot 10^{-7}$ (R; Ref. 11)	$1.1\cdot 10^{-7}$
289.2		$2.20\cdot 10^{-6}$ (D; Ref. 5)	$1.1\cdot 10^{-7}$
293.2		$2.00\cdot 10^{-7}$ (D; Ref. 3), $9.90\cdot 10^{-8}$ (T; Ref. 7)	$1.1\cdot 10^{-7}$
298.0	6500 (Ref. 10)	$1.40\cdot 10^{-7}$ (D; Ref. 10)	$1.0\cdot 10^{-7}$
298.2		$9.90\cdot 10^{-9}$ (D; Ref. 1), $9.70\cdot 10^{-8}$ (T; Ref. 7), $1.00\cdot 10^{-7}$ (R; Ref. 8), $1.04\cdot 10^{-7}$ (R; Ref. 9), $1.34\cdot 10^{-7}$ (D; Ref. 12), $6.80\cdot 10^{-8}$ (D; Ref. 13), $1.75\cdot 10^{-7}$ (D; Ref. 15)	$1.0\cdot 10^{-7}$
303.2		$9.60\cdot 10^{-8}$ (T; Ref. 7)	$1.0\cdot 10^{-7}$
308.2		$9.80\cdot 10^{-8}$ (T; Ref. 7)	$1.0\cdot 10^{-7}$
310.9	10.3 (Ref. 6)	$1.2\cdot 10^{-7}$ (T; Ref. 6)	$1.0\cdot 10^{-7}$
313.3		$8.26\cdot 10^{-8}$ (T; Ref. 13)	$1.0\cdot 10^{-7}$
318.2		$2.90\cdot 10^{-7}$ (D; Ref. 11)	$1.1\cdot 10^{-7}$
323.0	6500 (Ref. 10)	$2.00\cdot 10^{-7}$ (D; Ref. 10)	$1.1\cdot 10^{-7}$
342.9		$1.43\cdot 10^{-7}$ (T; Ref. 13)	$1.5\cdot 10^{-7}$
366.5	117 (Ref. 6)	$4.8\cdot 10^{-7}$ (D; Ref. 6)	$2.6\cdot 10^{-7}$
372.3		$1.77\cdot 10^{-7}$ (D; Ref. 13)	$3.1\cdot 10^{-7}$
373.0	6500 (Ref. 10)	$7.20\cdot 10^{-7}$ (D; Ref. 10)	$3.2\cdot 10^{-7}$
394.5		$7.29\cdot 10^{-7}$ (T; Ref. 13)	$6.3\cdot 10^{-7}$
409.8		$1.34\cdot 10^{-6}$ (T; Ref. 13)	$1.1\cdot 10^{-6}$
422.0	655 (Ref. 6)	$3.8\cdot 10^{-6}$ (D; Ref. 6)	$1.8\cdot 10^{-6}$
422.7		$1.86\cdot 10^{-6}$ (T; Ref. 13)	$1.9\cdot 10^{-6}$
423.0	6500 (Ref. 10)	$4.40\cdot 10^{-6}$ (D; Ref. 10)	$1.9\cdot 10^{-6}$
473.0	6500 (Ref. 10)	$2.90\cdot 10^{-5}$ (D; Ref. 10)	$1.7\cdot 10^{-5}$
479.5	2510 (Ref. 6)	$4.0\cdot 10^{-5}$ (D; Ref. 6)	$2.3\cdot 10^{-5}$
536.1	7030 (Ref. 6)	$3.5\cdot 10^{-4}$ (T; Ref. 6)	$3.5\cdot 10^{-4}$
552.8	8860 (Ref. 6)	$6.0\cdot 10^{-4}$ (T; Ref. 6)	$8.0\cdot 10^{-4}$

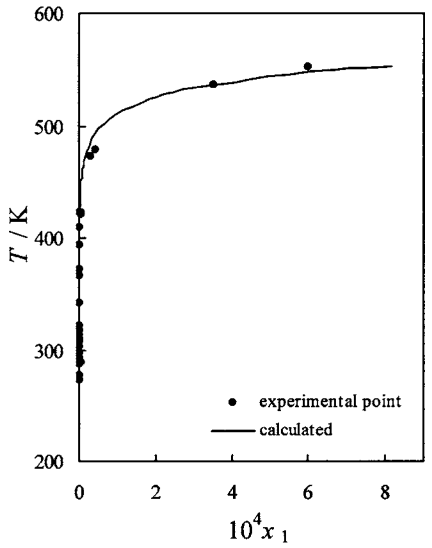

FIG. 5. All the solubility data for octane (1) in water (2).

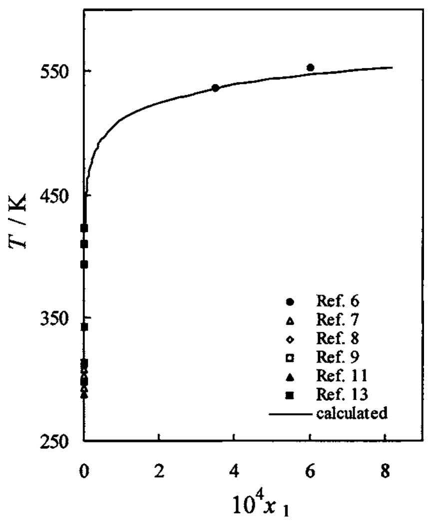

FIG. 6. Recommended and tentative solubility data for octane (1) in water (2).

TABLE 7. The data categories for solubility of water (2) in octane (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		Polak and Lu[12]	
283.2		Englin *et al.*[4]	
293.2		Budantseva *et al.*[3] Englin *et al.*[4]	Black *et al.*[2]
298.2		Polak and Lu[12]	
303.2			Englin *et al.*[4]
310.9		Heidman[6]	
366.5		Heidman[6]	
422.0		Heidman[6]	
477.6		Heidman[6]	
533.1		Heidman[6]	
539.1		Heidman[6]	
550.4		Heidman[6]	

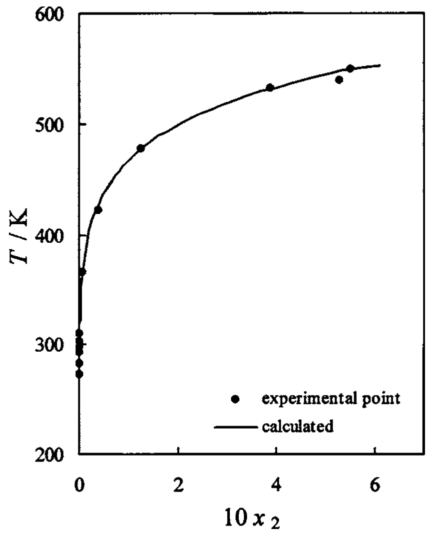

FIG. 7. All the solubility data for water (2) in octane (1).

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

T/K	P/kPa	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2		$1.46\cdot 10^{-4}$ (T; Ref. 12)	$2.0\cdot 10^{-4}$
283.2		$3.24\cdot 10^{-4}$ (T; Ref. 4)	$3.2\cdot 10^{-4}$
293.2		$9.00\cdot 10^{-4}$ (D; Ref. 2), $4.30\cdot 10^{-4}$ (T; Ref. 3), $6.03\cdot 10^{-4}$ (T; Ref. 4)	$4.9\cdot 10^{-4}$
298.2		$5.01\cdot 10^{-4}$ (T; Ref. 12)	$6.1\cdot 10^{-4}$
303.2		$1.065\cdot 10^{-3}$ (D; Ref. 4)	$7.5\cdot 10^{-4}$
310.9	10.3 (Ref. 6)	$1.00\cdot 10^{-3}$ (T; Ref. 6)	$1.0\cdot 10^{-3}$
366.5	117 (Ref. 6)	$6.20\cdot 10^{-3}$ (T; Ref. 6)	$7.2\cdot 10^{-3}$
422.0	655 (Ref. 6)	$3.94\cdot 10^{-2}$ (T; Ref. 6)	$3.4\cdot 10^{-2}$
477.6		$1.26\cdot 10^{-1}$ (T; Ref. 6)	$1.3\cdot 10^{-1}$
533.1		$3.87\cdot 10^{-1}$ (T; Ref. 6)	$4.0\cdot 10^{-1}$
539.1	7410 (Ref. 6)	$5.27\cdot 10^{-1}$ (T; Ref. 6)	$4.5\cdot 10^{-1}$
550.4		$5.49\cdot 10^{-1}$ (T; Ref. 6)	$5.7\cdot 10^{-1}$

Components:

(1) Octane; C_8H_{18} ; [111-65-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. G. Baker, Geochim. Cosmochim. Acta **19**, 309 (1960).

Variables:

One temperature: not specified

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of octane in water was reported to be $0.09 \cdot 10^{-6}$ mL(1)/mL(2).

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined after ultrafiltration using the procedure described in Baker.[1]

Source and Purity of Materials:

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

Estimated Error:

Not specified.

References:

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

Components:

(1) Octane; C_8H_{18} ; [111-65-9]
(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:

One temperature: 20 °C

Prepared By:

M.C. Haulait-Pirson

Experimental Values

The solubility of water in octane at 20 °C and at a total saturation pressure of 1 atm was reported to be 0.0142g(2)/100 g(1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.0142 g(2)/100 g sln and $9.0 \cdot 10^{-4}$.

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 in 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) Octane; C_8H_{18}; [111-65-9] (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. 1976, VINITI 438-76.
Variables:	**Prepared By:**
One temperature: 20 °C	A. Maczynski

Experimental Values

The solubility of octane in water at 20 °C was reported to be x_1 about $2 \cdot 10^{-7}$. The corresponding mass percent calculated by the compiler is about 0.0001 $g(1)$/100 g sln.

The solubility of water in octane at 20 °C was reported to be $x_2 = 4.3 \cdot 10^{-4}$. The corresponding mass percent value calculated by the compiler is 0.007 (2)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
Nothing specified in the paper.	(1) Not specified. (2) Not specified. **Estimated Error:** Not specified.

Components:	**Original Measurements:**
(1) Octane; C_8H_{18}; [111-65-9] (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: 10–30 °C	A. Maczynski and M C. Haulait-Pirson

Experimental Values

Solubility of water in octane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.24	0.0051
20	6.03	0.0095
30	10.65	0.0168

Auxiliary Information

Method/Apparatus/Procedure:	**Source and Purity of Materials:**
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) Not specified. (2) Not specified. **Estimated Error:** Not specified.

Components:
(1) Octane; C_8H_{18}; [111-65-9]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 16 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of octane in water at 16 °C was reported to be 0.002 mL (1)/100 mL sln or 0.0014 $g(1)/100$ g sln. The corresponding mole fraction, x_1, calculated by the compiler is $0.22\cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a stoppered measuring 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 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) Octane; C_8H_{18}; [111-65-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

Variables:
Temperature: 311–553 K
Pressure: 0.01–7.4 MPa

Prepared By:
G. T. Hefter

Experimental Values

Solubility of octane in water

T/K	$10^5\cdot x_1$	$10^2\cdot g(1)/100$ g sln (compiler)	P/MPa
310.9	0.012	0.0076	0.0103[a]
366.5	0.048	0.030	0.117[a]
422.0	0.38	0.24	0.655
479.5	4.0	2.5	2.51
536.1	35	22	7.03
552.8	60[b]	38	8.86

[a] Estimated by the authors from pure component data.
[b] Above three-phase equilibrium point.

Solubility of water in octane

T/K	$10^2\cdot x_2$	$g(2)/100$ g sln (compiler)	P/MPa
310.9	0.100	0.0158	0.0103[a]
366.5	0.62	0.098	0.117
422.0	3.94	0.622	0.655
477.6	12.6	2.22	—[b]
533.1	38.7	9.05	—[b]
539.1[c]	52.7[c]	14.9	7.41
550.4[d]	54.9[d]	16.1	—

[a] Estimated by the authors from pure component data.
[b] Not specified.
[c] Three phase critical point.
[d] Above three phase critical point.

The three phase critical point was reported to be 539.1 ± 0.6 K, 7.37 ± 0.04 MPa, and $x_1=4.61\cdot 10^{-4}$ ($0.292\ g(1)/100$ g sln, compiler).

The authors also report an equation which fit their own and literature data over the range 273–539 K, viz.

$$\ln x_1=-343.1497+13862.49/T+49.24609\ln T$$

$$\ln x_2=-0.66037-7.1130(T_r^{-1}-1)-0.67885(1-T_r)^{1/3}-1.43381(1-T_r)$$

where $T_r=T/539.1$.

Auxiliary Information

Method/Apparatus/Procedure:

Experimental procedure was similar to that used in Ref. 1. Hydrocarbons were determined by gas chromatography and water by the Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.

Source and Purity of Materials:

(1) Aldrich 99+ mol %; water free purity greater than or equal to 99.9 mol %, checked by gas chromatography.
(2) Distilled; no details given.

Estimated Error:

Temperature: not stated.
Solubility: ±5%, relative precision of replicate analyses.
Pressure: ±1%; type of error not stated.

References:

[1] C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).

Components:

(1) Octane; C_8H_{18} ; [111-65-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. A. Jonsson, J. Vejrosta, and J. Novak, Fluid Phase Equilib. **9**, 279 (1982).

Variables:

Temperature: 15–35 °C

Prepared By:

G. T. Hefter

Experimental Values

Solubility of octane in water

t/°C	$10^7 \cdot x_1$ (compiler)	10^5 $g(1)$/100 g sln (compiler)	mg (1)/kg sln
15	1.03	6.53	0.653
20	0.99	6.28	0.628
25	0.97	6.15	0.615
30	0.96	6.12	0.612
35	0.98	6.20	0.620

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

Auxiliary Information

Method/Apparatus/Procedure:

Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapor concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and 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, >99.8%, used as received.
(2) Not specified.

Estimated Error:

Not specified.

References:

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

Components:

(1) Octane; C_8H_{18}; [111-65-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski

Experimental Values

The solubility of octane in water at 25 °C was reported to be $x_1 = 1.0 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $7.0 \cdot 10^{-5}$ $g(1)$/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) Octane; C_8H_{18}; [111-65-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of octane in water at 25 °C was reported to be 0.66 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is $1.04 \cdot 10^{-7}$. The same value is also reported in two references.[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 mL 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: 0.06 mg (1)/kg sln (std. dev. from mean).

References:

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

Components:

(1) Octane; C_8H_{18}; [111-65-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 298.0–473.0 K
Pressure: 65 bar

Prepared By:

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

Experimental Values

Solubility of octane in water

T/K	P/bar	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
298.0	65	$8.88 \cdot 10^{-5}$	0.014±0.002
323.0	65	$1.27 \cdot 10^{-4}$	0.020±0.004
373.0	65	$4.57 \cdot 10^{-4}$	0.072±0.002
423.0	65	$2.79 \cdot 10^{-3}$	0.44±0.02
473.0	65	$1.84 \cdot 10^{-2}$	2.9±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 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) Octane; C_8H_{18}; [111-65-9]
(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: 5–45 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

Solubility of octane in water

t/°C	$10^7 \cdot x_1$	mg (1)/kg sln (compiler)
5.0	2.6±0.6	1.65
15.0	1.4±0.6	0.89
45.0	2.9±0.6	1.84

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 the septum and injected into the gas chromatograph equipped with a flame ionization detector. The gas chromatographic conditions are described in the paper.

Source and Purity of Materials:

(1) Fluka purum.
(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 (standard deviation).

Components:	**Original Measurements:**
(1) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O; [7732-18-5]	J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).
Variables:	**Prepared By:**
Temperature: 0–25 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of octane in water

t/°C	$10^7 \cdot x_1$ (compiler)	mg (1)/kg sln
0^a	2.13	1.35^c
25^b	1.34	0.85^c

Solubility of water in octane

t/°C	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0^a	1.46	23^d
25^b	5.01	79^e

[a–e] See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:

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

Components:	**Original Measurements:**
(1) Octane; C_8H_{18} ; [111-65-9] (2) Water; H_2O; [7732-18-5]	L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
Variables:	**Prepared By:**
Temperature: 25–149.5 °C	F. Kapuku

Experimental Values

Solubility of octane in water

t/°C	mg (1)/kg (2)	$g(1)$/100 g sln (compiler)	$10^7 \cdot x_1$ (compiler)
25.0	0.431±0.012	0.0000431	0.680
40.1	0.524±0.021	0.0000524	0.826
69.7	0.907±0.042	0.0000907	1.43
99.1	1.12±0.07	0.000112	1.77
121.3	4.62±0.22	0.000462	7.29
136.6	8.52±0.34	0.000852	13.4
149.5	11.89±0.7	0.00118	18.6

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 cylinders 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; purity 99+%; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: range of values given above.

Components:

(1) Octane; C_8H_{18}; [111-65-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skripka, Tr., Vses. Neftegazov. Nauch.-Issled. Inst. **61**, 139 (1976).
R. G. Sultanov and V. E. Skripka, Zh. Fiz. Khim. **47**, 1035 (1973).

Variables:

Temperature: 225–265 °C
Pressure: 3.5–78.5 MPa

Prepared By:

A. Maczynski

Experimental Values

Solubility of octane in water

$t/°C$	x_2	$g(2)/100$ g sln (compiler)	$P/\mathrm{kg \cdot cm^{-2}}$	P/MPa (compiler)
225	0.166	3.04	36	3.5
	0.137	2.44	100	9.8
	0.109	1.89	200	19.6
	0.098	1.68	300	29.4
	0.091	1.55	400	39.2
	0.088	1.50	500	49.0
	0.084	1.42	600	58.8
	0.080	1.35	700	68.6
	0.075	1.26	800	78.5
240	0.216	4.16	50	4.9
	0.193	3.63	100	9.8
	0.164	3.00	200	19.6
	0.149	2.69	300	29.4
	0.140	2.50	400	39.2
	0.132	2.34	500	49.0
	0.126	2.22	600	58.8
	0.122	2.14	700	68.6
	0.117	2.05	800	78.5
265	0.412	9.95	75	7.4
	0.350	7.83	100	9.8
	0.254	5.10	200	19.6
	0.224	4.35	300	29.4
	0.207	3.95	400	39.2
	0.194	3.66	500	49.0
	0.183	3.41	600	58.8
	0.172	3.19	700	68.6
	0.163	2.98	800	78.5

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Not specified.

References:

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

Components:

(1) Octane; C_8H_{18}; [111-65-9]
(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 Values

Solubility of octane in water

$t/°C$	mol (1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
25.0	$9.66 \cdot 10^{-6}$	$1.107 \cdot 10^{-4}$	$1.745 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

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

References:

[1] H. 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).

2.19. 2,2,4-Trimethylpentane+Water

Components:	Evaluators:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

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

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

Author (s)	T/K	Author (s)	T/K
Baker[1]	298	Miller and Hawthorne[7]	298–473 K (6500 kPa)
Budantseva *et al.*[3]	293	Polak and Lu[9]	273 and 298
McAuliffe[6]	298	Price[10]	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:

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

where $\ln x_{\min,1}=-15.33$, $\Delta_{\rm sln}C_p/R=57.3$, 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.

All the experimental and reference data are listed in Table 9 and shown in Fig. 8. The data of Budantseva *et al.*[3] at 293 K, Polak and Lu[9] at 273 K and 298 K, and Price[10] at 298 K are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Baker,[1] McAuliffe,[6] and Miller and Hawthorne[7] 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 2,2,4-Trimethylpentane (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
Berkengeim[2]	271–313	Gramajo de Doz *et al.*[5]	303
Budantseva *et al.*[3]	293	Peschke and Sandler[8]	298
Englin *et al.*[4]	273–323	Polak and Lu[9]	273 and 298

TABLE 9. Experimental values for solubility of 2,2,4-trimethylpentane (1) in water (2)

T/K	P/kPa	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2		$3.88\cdot10^{-7}$(T; Ref. 9)	$3.6\cdot10^{-7}$
293.2		$3.0\cdot10^{-7}$ (T; Ref. 3)	$2.6\cdot10^{-7}$
298.0	6500 (Ref. 7)	$3.50\cdot10^{-7}$ (D; Ref. 7), $4.40\cdot10^{-7}$ (D; Ref. 7)	$2.5\cdot10^{-7}$
298.2		$9.80\cdot10^{-8}$ (D; Ref. 1), $3.85\cdot10^{-7}$ (D; Ref. 6), $3.23\cdot10^{-7}$ (T; Ref. 9), $1.80\cdot10^{-7}$ (T; Ref. 10)	$2.5\cdot10^{-7}$
323.0	6500 (Ref. 7)	$5.20\cdot10^{-7}$ (D; Ref. 7)	$2.7\cdot10^{-7}$
373.0	6500 (Ref. 7)	$2.00\cdot10^{-6}$ (D; Ref. 7)	$7.1\cdot10^{-7}$
423.0	6500 (Ref. 7)	$1.02\cdot10^{-5}$ (D; Ref. 7)	$3.7\cdot10^{-6}$
473.0	6500 (Ref. 7)	$6.10\cdot10^{-5}$ (D; Ref. 7)	$2.8\cdot10^{-5}$

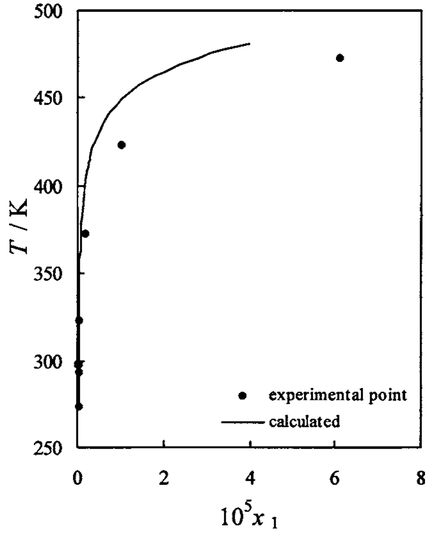

FIG. 8. All the solubility data for 2,2,4-trimethylpentane (1) in water (2).

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 $d_1=-0.499$, $d_2=-6.314$, $d_3=-0.954$, $d_4=-2.859$, and $T_r=T/526.7$.

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

The experimental and reference solubility data for (2) in (1) are listed in Table 10 and shown in Fig. 9. The data of Budantseva *et al.*[3] at 293 K, Englin *et al.*[4] at 273 and 283 K, and Polak and Lu[9] at 273 and 298 K are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. All the remaining data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

TABLE 10. Experimental values for solubility of water (2) in 2,2,4-trimethylpentane (1)

T/K	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
271.7	$6.97\cdot10^{-5}$ (D; Ref. 2)	$1.9\cdot10^{-4}$
273.2	$1.97\cdot10^{-4}$ (T; Ref. 4), $1.46\cdot10^{-4}$ (T; Ref. 9)	$2.1\cdot10^{-4}$
283.2	$2.35\cdot10^{-4}$ (D; Ref. 2), $3.74\cdot10^{-4}$ (T; Ref. 4)	$3.4\cdot10^{-4}$
293.2	$3.49\cdot10^{-4}$ (D; Ref. 2), $4.4\cdot10^{-4}$ (T; Ref. 3), $7.29\cdot10^{-4}$ (D; Ref. 4)	$5.4\cdot10^{-4}$
298.2	$3.6\cdot10^{-3}$ (D; Ref. 8), $5.07\cdot10^{-4}$ (T; Ref. 9)	$6.7\cdot10^{-4}$
303.2	$1.274\cdot10^{-3}$ (D; Ref. 4), $3.8\cdot10^{-3}$ (D; Ref. 5)	$8.4\cdot10^{-4}$
313.2	$5.07\cdot10^{-4}$ (D; Ref. 2), $2.102\cdot10^{-3}$ (D; Ref. 4)	$1.3\cdot10^{-3}$
323.2	$3.403\cdot10^{-3}$ (D; Ref. 4)	$1.9\cdot10^{-3}$

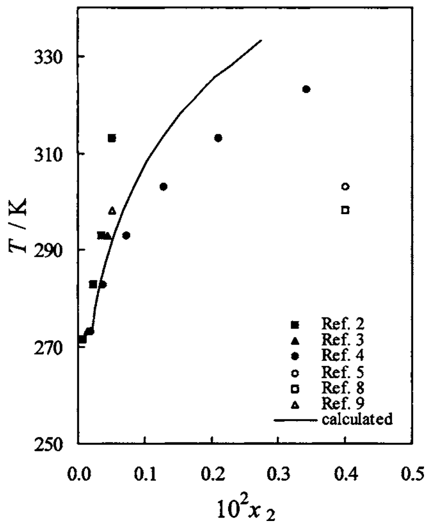

FIG. 9. All the solubility data for water (2) in 2,2,4-trimethylpentane (1).

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[11] are independent data. Therefore these data are Rejected.

References:

[1] E. G. Baker, Geochim. Cosmochim. Acta **19**, 309 (1960).
[2] T. I. Berkengeim, Zavod. Lab. **10**, 592 (1941).
[3] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).
[4] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[5] M. B. Gramajo de Doz, C. M. Bonatti, N. Solimo, and H. N. Barnes, J. Chem. Thermodyn. **33**, 1663 (2001).
[6] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[7] D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).
[8] N. Peschke and S. I. Sandler, J. Chem. Eng. Data **40**, 315 (1995).
[9] J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[10] L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[11] T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Components:
(1) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. G. Baker, Geochim. Cosmochim. Acta **19**, 309 (1960).

Variables:
One temperature: not specified

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 2,2,4-trimethylpentane in water was reported to be 0.0009 mL (1)/L (2).

Auxiliary Information

Method/Apparatus/Procedure:
The procedure is described in Baker.[1]

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

Estimated Error:
Not specified.

References:
[1] E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Preprints C61 **4**, 3 (1958).

Components:
(1) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. I. Berkengeim, Zavod. Lab. **10**, 592 (1941).

Variables:
Temperature: (−1.5)–40 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of water in 2,2,4-trimethylpentane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
−1.5	0.697	0.0011
10	2.35	0.0037
20	3.49	0.0055
40	5.07	0.0080

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (2) in (1) was determined by the Karl Fischer method.

Source and Purity of Materials:
(1) Source not specified; CP reagent; d^{20} 0.6947; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of 2,2,4-trimethylpentane in water at 20 °C was reported to be $x_1 = 3 \cdot 10^{-7}$. The corresponding mass percent calculated by the compiler is about $2 \cdot 10^{-4}$ $g(1)$/100 g sln.

The solubility of water in 2,2,4-trimethylpentane at 20 °C was reported to be $x_2 = 4.4 \cdot 10^{-4}$. The corresponding mass percent value calculated by the compiler is $7.9 \cdot 10^{-3}(2)$/100 g sln.

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:

(1) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 0–50 °C

Prepared By:

A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in 2,2,4-trimethylpentane

$t/°C$	$10^4 \cdot x_2$ (compiler)	$g(2)/100$ g sln
0	1.97	0.0031
10	3.74	0.0059
20	7.29	0.0115
30	12.74	0.0201
40	21.02	0.0332
50	34.03	0.0538

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) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. B. Gramajo de Doz, C. M. Bonatti, N. Barnes, and H. N. Solimo, J. Chem. Thermodyn. **33**, 1663 (2001).

Variables:

One temperature: 303.15 K

Prepared By:

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

Experimental Values

Solubility of water in 2,2,4-trimethylpentane

T/K	$g(2)/100$ g sln	x_2 (compilers)
303.15	0.06	0.0038

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Mixtures of known overall composition were prepared in 16 mL vials, intensively stirred for at least 7 days in water bath and then allowed to settle for 24 h. The both phases were analyzed chromatographically (Hewlett Packard 6890 apparatus connected to a ChemStation HP G2070AA). The internal standard method was applied. Three or four analyses were performed for each sample.

Source and Purity of Materials:

(1) Fluka, pure for analysis grade; purity checked by glc >99.8 mass %; used as received.
(2) Twice distilled.

Estimated Error:

Temperature: ±0.05 K.
Solubility: >1% (reproducibility).

Components:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 2,2,4-trimethylpentane in water at 25 °C was reported to be 2.44 mg (1)/kg sln.
The corresponding mole fraction, x_1, calculated by the compiler, is $3.85 \cdot 10^{-7}$. The same value is also reported in 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 mL 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: 0.12 mg (1)/kg sln (std. dev. from mean).

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

Components:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 298.0–473.0 K
Pressure: 65 bar

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

Experimental Values

Solubility of 2,2,4-trimethylpentane in water

T/K	P/bar	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
298.0	65	0.000279	0.044±0.005
323.0	65	0.000330	0.052±0.004
373.0	65	0.00127	0.20±0.01
423.0	65	0.00647	1.02±0.03
473.0	65	0.0387	6.1±0.3

Auxiliary Information

Method/Apparatus/Procedure:
The dynamic method described by 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. **78**, 1618 (1998).

Components:

(1) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]
(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 Values

Solubility of water in 2,2,4-trimethylpentane

$t/°C$	$g(2)/100$ g sln (compilers)	x_2
25.0	0.057	0.0036

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 99.7 mass %; used as received.
(2) Deionized water.

Estimated Error:

Temperature: ±0.1°C.

Components:

(1) 2,2,4-Trimethylpentane; C_8H_{18} ; [540-84-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 0–25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

Solubility of 2,2,4-trimethylpentane in water

$t/°C$	$10^7 \cdot x_1$ (compiler)	mg (1)/kg sln
0^a	3.88	2.46^c
25^b	3.23	2.05^c

Solubility of water in 2,2,4-trimethylpentane

$t/°C$	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0^a	1.46	23^d
25^b	5.07	80^e

[a–e] See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:

Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±4%, (d) ±4.7%, (e) ±3.1% (mean from two or three determinations).

Components:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of 2,2,4-trimethylpentane in water at 25 °C and at system pressure was reported to be 1.14 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $1.14\cdot 10^{-4}$ $g(1)/100$ g sln and $1.80\cdot 10^{-7}$.

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).

2.20. 2,3,4-Trimethylpentane+Water

Components:

(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3]
(2) Water; H_2O; [7732-18-5]

Evaluators:

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

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

The experimental solubility for (1) in (2) has been investigated by Polak and Lu[1] at 273 K 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 $\ln x_{\min,1} = -15.11$, $\Delta_{\text{sln}}C_p/R = 56.2$, and $T_{\min} = 306$ K.

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

All the experimental and reference data are listed in Table 11. The data of Polak and Lu[1] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Price[2] 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 2,3,4-Trimethylpentane (1)

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

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

where $d_1 = -0.466$, $d_2 = -5.950$, $d_3 = -0.968$, $d_4 = -3.034$, and $T_r = T/541.6$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 2,3,4-trimethylpentane 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 good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[3] are independent data. Therefore these data are Rejected.

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

T/K	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$3.69\cdot 10^{-7}$ (T; Ref. 1)	$4.5\cdot 10^{-7}$
298.2	$3.62\cdot 10^{-7}$ (T; Ref. 1), $2.14\cdot 10^{-7}$ (D; Ref. 2)	$3.2\cdot 10^{-7}$

TABLE 12. Experimental values for solubility of water (2) in 2,3,4-trimethylpentane (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
273.2	$1.27\cdot 10^{-4}$ (T; Ref. 1)	$1.9\cdot 10^{-4}$
298.2	$4.69\cdot 10^{-4}$ (T; Ref. 1)	$5.9\cdot 10^{-4}$

Components:

(1) 2,3,4-Trimethylpentane; C_8H_{18} ; [565-75-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 0–25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

Solubility of 2,3,4-trimethylpentane in water

t/°C	$10^7 \cdot x_1$ (compiler)	mg (1)/kg sln
0^a	3.69	2.34^c
25^b	3.62	2.30^c

Solubility of water in 2,3,4-trimethylpentane

t/°C	$10^4 \cdot x_2$ (compiler)	mg (2)/kg sln
0^a	1.27	20^d
25^b	4.69	74^e

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:

Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±4%, (d) ±4.7%, (e) ±3.1% (mean from two or three determinations).

Components:

(1) 2,3,4-Trimethylpentane; C_8H_{18} ; [565-75-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Values

The solubility of 2,3,4-trimethylpentane in water at 25 °C and at system pressure was reported to be 1.36 mg (1)/kg (2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $1.36 \cdot 10^{-4}$ $g(1)/100$ g sln and $2.14 \cdot 10^{-7}$.

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: ±0.03 mg(1)/kg(2).

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.