IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater-Revised and Updated. Part 5. C₇ Hydrocarbons with Water and Heavy Water

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The mutual solubility and related liquid-liquid equilibria of C7 hydrocarbons with water and heavy water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 23 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For 9 systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of all experimental data for a given homologous series of aliphatic and aromatic hydrocarbons was used. © 2005 American Institute of Physics.

Key words: C7 hydrocarbons; critical evaluation; heavy water; liquid-liquid equilibria; solubility; water

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1. Preface

1.1. Scope of this Volume

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

This revised work also includes all new evaluations for systems where two or more independent measurements of solubility have been reported. In these evaluations, reported solubility values are characterized as Recommended, Tentative, Doubtful, or Rejected, based on consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.3–6 Recommended values are supported by two (or more) independent experimental values and a reference value that are all in agreement. Tentative values are supported by two (or more) independent values in agreement with each other, but not with the reference value, or one experimental value in agreement with the reference value. Doubtful values are those for which a single experimental value differs from the reference value. Experimental values that differ from reference values and other experimental values are Rejected.

Detailed introductory material including explanations of the formats of compilation and evaluation, definitions of commonly used measures of solubility, and the scope of the Solubility Data Series can be found in Part 1 (Maczynski and Shaw7) The derivation of the smoothing equations used to calculate reference values can be found in Parts 1 and 2 (Maczynski and Shaw7,8).

1.2. References for the Preface

2. C₇ Hydrocarbons with Water and Heavy Water

2.1. 1,3,5-Cycloheptatriene+Water

Components:
(1) 1,3,5-Cycloheptatriene; C₇H₈ [544-25-2]  
(2) Water; H₂O; [7732-18-5]

Evaluators:

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

The experimental solubility data for (1) in (2) have been investigated by McAuliffe² at 298 K and Pierotti and Liabastre³ at 278 K–318 K.

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

\[ \ln x_1 = \ln x_{1\text{ref}} + (\Delta x_1 C_p \{ R[T_{\text{ref}} - \ln(T_{\text{ref}}/T)] - 1 \} ) \]

where \( \ln x_{1\text{ref}} = -9.09 \), \( \Delta x_1 C_p / R = 37.1 \), and \( T_{\text{ref}} = 298 \) K.

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

The experimental and reference data of McAuliffe,² and Pierotti and Liabastre³ are listed in Table 1. Since only one experimental data point is available at each temperature, no data can be Recommended. The data of McAuliffe² and Pierotti and Liabastre³ in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

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

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

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

\[ \ln x_2 = d_1 + d_2 (1/T - 1) + d_3 (1 - T/T_0)^{1/3} + d_4 (1 - T_0) \]

where \( d_1 = 0.489 \), \( d_2 = -1.227 \), \( d_3 = -1.196 \), \( d_4 = -8.963 \), and \( T_0 = 7558.3 \) K.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1,3,5-cycloheptatriene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 2. All the data are in good agreement with the reference data and are Tentative.

References:

---

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

<table>
<thead>
<tr>
<th>( T/K )</th>
<th>( x_1 ) (( T = \text{tentative} ))</th>
<th>( x_1 \pm \text{30%} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>278.3</td>
<td>1.136 ( \times ) 10⁻⁴ (T; Ref. 3)</td>
<td>1.2 ( \times ) 10⁻⁴</td>
</tr>
<tr>
<td>288.4</td>
<td>1.299 ( \times ) 10⁻⁴ (T; Ref. 3)</td>
<td>1.2 ( \times ) 10⁻⁴</td>
</tr>
<tr>
<td>298.2</td>
<td>1.21 ( \times ) 10⁻⁴ (T; Ref. 2)</td>
<td>1.1 ( \times ) 10⁻⁴</td>
</tr>
<tr>
<td>298.3</td>
<td>1.309 ( \times ) 10⁻⁴ (T; Ref. 3)</td>
<td>1.1 ( \times ) 10⁻⁴</td>
</tr>
<tr>
<td>308.4</td>
<td>1.45 ( \times ) 10⁻⁴ (T; Ref. 3)</td>
<td>1.2 ( \times ) 10⁻⁴</td>
</tr>
<tr>
<td>318.4</td>
<td>1.495 ( \times ) 10⁻⁴ (T; Ref. 3)</td>
<td>1.2 ( \times ) 10⁻⁴</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>( T/K )</th>
<th>( x_2 ) (( T = \text{tentative} ))</th>
<th>( x_2 \pm \text{30%} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>303.2</td>
<td>3.21 ( \times ) 10⁻³ (T; Ref. 1)</td>
<td>3.8 ( \times ) 10⁻³</td>
</tr>
<tr>
<td>313.2</td>
<td>3.94 ( \times ) 10⁻³ (T; Ref. 1)</td>
<td>4.9 ( \times ) 10⁻³</td>
</tr>
<tr>
<td>323.2</td>
<td>5.06 ( \times ) 10⁻³ (T; Ref. 1)</td>
<td>6.2 ( \times ) 10⁻³</td>
</tr>
<tr>
<td>Temperature</td>
<td>$10^3 x_1$ (compiler)</td>
<td>g/(2)/100 g sln</td>
</tr>
<tr>
<td>-------------</td>
<td>----------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>30</td>
<td>3.21</td>
<td>0.0630</td>
</tr>
<tr>
<td>40</td>
<td>3.94</td>
<td>0.0773</td>
</tr>
<tr>
<td>50</td>
<td>5.06</td>
<td>0.0993</td>
</tr>
</tbody>
</table>

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

Estimated Error:
Not specified.
2.2. 1,6-Heptadiyne + Water

Components:
(1) 1,6-Heptadiyne; C₇H₈; [2396-63-6]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C

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

Experimental Data
The solubility of 1,6-heptadiyne in water at 25 °C was reported to be 1650 mg (1)/100 g sln.
The corresponding mass percent and mole fraction, x₁, calculated by the compilers are 0.1650 g(1)/100 g sln and 3.23 × 10⁻⁴.

Auxiliary Information

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

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

Estimated Error:
Temperature: ± 1.5 °C.
Solubility: 25 mg (1)/100 g (2) standard deviation of the mean.
**2.3. 2,5-Norbornadiene+Water**

Components:
1. 2,5-Norbornadiene; C<sub>7</sub>H<sub>8</sub>; [121-46-0]
2. Water; H<sub>2</sub>O; [7732-18-5]

Original Measurements:

Variables:
Temperature: 20 °C–50 °C

Prepared By:
A. Maczynski and Z. Maczynska

### Experimental Data

**Solubility of water in 2,5-norbornadiene**

<table>
<thead>
<tr>
<th>T/°C</th>
<th>x&lt;sub&gt;2&lt;/sub&gt; (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.51</td>
<td>0.0295</td>
</tr>
<tr>
<td>30</td>
<td>1.96</td>
<td>0.0383</td>
</tr>
<tr>
<td>50</td>
<td>3.44</td>
<td>0.0675</td>
</tr>
</tbody>
</table>

**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.

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

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

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Author(s)</th>
<th>T/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anderson and Prausnitz</td>
<td>373–474</td>
<td>Mackay and Shin</td>
<td>298</td>
</tr>
<tr>
<td>Andrews and Keefer</td>
<td>298</td>
<td>McAuliffe</td>
<td>38</td>
</tr>
<tr>
<td>Ben-Naim and Wolff</td>
<td>283–293</td>
<td>Miller and Hawthorne</td>
<td>41</td>
</tr>
<tr>
<td>Ben-Naim and Wolff</td>
<td>298</td>
<td>McAuliffe</td>
<td>39</td>
</tr>
<tr>
<td>Bohon and Claussen</td>
<td>298</td>
<td>Polak and Lu</td>
<td>45</td>
</tr>
<tr>
<td>Booth and Everson</td>
<td>298</td>
<td>Price</td>
<td>46</td>
</tr>
<tr>
<td>Bradley et al</td>
<td>298–328</td>
<td>Rossi and Thomas</td>
<td>46</td>
</tr>
<tr>
<td>Brown et al</td>
<td>341–324</td>
<td>Sada et al</td>
<td>50</td>
</tr>
<tr>
<td>Brown and Wasik</td>
<td>278–293</td>
<td>Sanemasa et al</td>
<td>50</td>
</tr>
<tr>
<td>Chandler et al</td>
<td>473–548</td>
<td>Sanemasa et al</td>
<td>51</td>
</tr>
<tr>
<td>Chen and Wagner</td>
<td>303–373</td>
<td>Sanemasa et al</td>
<td>52</td>
</tr>
<tr>
<td>Chey and Calder</td>
<td>294</td>
<td>Sanemasa et al</td>
<td>53</td>
</tr>
<tr>
<td>Dohnanyova et al</td>
<td>274–328</td>
<td>Sawamura et al</td>
<td>54</td>
</tr>
<tr>
<td>Fühner</td>
<td>289</td>
<td>Sawamura et al</td>
<td>55</td>
</tr>
<tr>
<td>Gross and Saykoe</td>
<td>303</td>
<td>Schwarz</td>
<td>289</td>
</tr>
<tr>
<td>Gusyev and Pamon</td>
<td>360–480</td>
<td>Schwarz and Miller</td>
<td>283–303</td>
</tr>
<tr>
<td>Gusyev and Pamon</td>
<td>363–497</td>
<td>Stephenson</td>
<td>273–363</td>
</tr>
<tr>
<td>Keeley et al</td>
<td>298</td>
<td>Sutton and Calder</td>
<td>289</td>
</tr>
<tr>
<td>Kleven</td>
<td>298</td>
<td>Tamura et al</td>
<td>50</td>
</tr>
<tr>
<td>Korenman and Aref’eva</td>
<td>293</td>
<td>Tewari et al</td>
<td>82</td>
</tr>
<tr>
<td>Korenman and Aref’eva</td>
<td>298</td>
<td>Uspenskii</td>
<td>283–295</td>
</tr>
<tr>
<td>Krasnoschekova and Gubergits</td>
<td>298</td>
<td>Vesalä</td>
<td>289</td>
</tr>
<tr>
<td>Li et al</td>
<td>298</td>
<td>Wing and Johnston</td>
<td>289</td>
</tr>
<tr>
<td>Ma et al</td>
<td>278–318</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

\[
\ln x_2 = \ln x_{2\text{ref}} + \frac{D_1}{T_{\text{ref}}} \ln \left( T_{\text{ref}} / T \right) + 1 - \left( T_{\text{ref}} / T \right),
\]

where \( \ln x_{2\text{ref}} = -9.14, D_1 = 35.7 \), and \( T_{\text{ref}} = 290 \).

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in the Table 3.

All the experimental and reference data are listed in the Table 4 and shown in Fig. 1. The Recommended and Tentative data are shown in Fig. 2.
Critical Evaluation of the Solubility of Water (2) in Toluene (1)

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

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Author(s)</th>
<th>T/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anderson and Prausnitz</td>
<td>373–474 (153–2603 kPa)</td>
<td>Johnson et al.</td>
<td>298</td>
</tr>
<tr>
<td>Benenkovskii et al.</td>
<td>303</td>
<td>Jones and Monk</td>
<td>298–308</td>
</tr>
<tr>
<td>Brown et al.</td>
<td>422–524 (6800 kPa)</td>
<td>Peschke and Sandier</td>
<td>298</td>
</tr>
<tr>
<td>Caddick and Davies</td>
<td>293</td>
<td>Polak and Lu</td>
<td>273–298</td>
</tr>
<tr>
<td>Chen and Wagner</td>
<td>303–373 (100–350 kPa)</td>
<td>Rosenbaum and Walton</td>
<td>283–323</td>
</tr>
<tr>
<td>Chandler et al.</td>
<td>473–548 (2500–8600 kPa)</td>
<td>Stephenson</td>
<td>273–363</td>
</tr>
<tr>
<td>Englin et al.</td>
<td>273–323</td>
<td>Tamura et al.</td>
<td>298</td>
</tr>
<tr>
<td>Glasoe and Shultz</td>
<td>288–303</td>
<td>Tarasenson and Polosushkevich</td>
<td>264–366</td>
</tr>
<tr>
<td>Gregory et al.</td>
<td>298</td>
<td>Uspeeskii</td>
<td>283–295</td>
</tr>
<tr>
<td>Hsiehfeld and Bolander</td>
<td>298</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

$$
\ln x_2 = d_1 + d_2 \left(T - T_1 \right) + d_3 \left(T - T_1 \right)^2 + d_4 \left(T - T_1 \right)^3,
$$

where $d_1 = -0.495$, $d_2 = -3.70$, $d_3 = -1.02$, $d_4 = -4.641$, and $T_1 = 273.0 K$.

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

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

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

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

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Author(s)</th>
<th>T/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bradley et al.</td>
<td>298–328 (100 000 kPa)</td>
<td>Haruki et al.</td>
<td>573</td>
</tr>
<tr>
<td>Chandler et al.</td>
<td>523–548 (10 000 kPa)</td>
<td>Eger</td>
<td>423–573</td>
</tr>
<tr>
<td>Connolly et al.</td>
<td>553–583 (17 200 kPa)</td>
<td>Sawamura et al.</td>
<td>298</td>
</tr>
<tr>
<td></td>
<td>(14 700–60 800 kPa)</td>
<td></td>
<td>(25 000–40 000 kPa)</td>
</tr>
</tbody>
</table>

Rejected and Inaccessible Data

In the opinion of the Evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[66] are independent data. The data reported by Alwani and Schneider[55] Gill et al.[50] Tarasenson and Polosushkevich[59] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

Table 3. The data categories for solubility of toluene (1) in water (2)

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IUPAC-NIST SOLUBILITY DATA SERIES

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Fig. 1. All the solubility data for toluene (1) in water (2).
### Table 5. The data categories for solubility of water (2) in toluene (1)

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<td>Tarassenkow and Poloshinzewa\textsuperscript{61}</td>
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<td></td>
</tr>
<tr>
<td>293.2</td>
<td>Caddock and Davies\textsuperscript{13}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>295.2</td>
<td>Uspenskii\textsuperscript{63}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Fig. 2.** Recommended and tentative solubility data for toluene (1) in water (2).
<table>
<thead>
<tr>
<th>T/K</th>
<th>P/kPa</th>
<th>Experimental values for solubility of water (2) in toluene (1)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(R = recommended, T = tentative, D = doubtful)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Reference values $x_2 \pm 30%$</td>
</tr>
<tr>
<td>264.2</td>
<td>1.00 $\times 10^{-4}$ (D; Ref. 61)</td>
<td>8.7 $\times 10^{-4}$</td>
</tr>
<tr>
<td>269.7</td>
<td>3.00 $\times 10^{-4}$ (D; Ref. 61)</td>
<td>1.1 $\times 10^{-3}$</td>
</tr>
<tr>
<td>273.2</td>
<td>1.382 $\times 10^{-3}$ (T; Ref. 19), 1.17 $\times 10^{-3}$ (T; Ref. 45), 2.14 $\times 10^{-3}$ (D; Ref. 58)</td>
<td>1.2 $\times 10^{-3}$</td>
</tr>
<tr>
<td>282.7</td>
<td>2.91 $\times 10^{-3}$ (D; Ref. 58)</td>
<td>1.7 $\times 10^{-3}$</td>
</tr>
<tr>
<td>283.2</td>
<td>1.61 $\times 10^{-3}$ (R; Ref. 19), 1.71 $\times 10^{-3}$ (R; Ref. 47), 2.18 $\times 10^{-3}$ (T; Ref. 63)</td>
<td>1.7 $\times 10^{-3}$</td>
</tr>
<tr>
<td>283.7</td>
<td>1.00 $\times 10^{-3}$ (T; Ref. 61)</td>
<td>1.7 $\times 10^{-3}$</td>
</tr>
<tr>
<td>288.2</td>
<td>2.11 $\times 10^{-3}$ (T; Ref. 21), 1.71 $\times 10^{-3}$ (T; Ref. 21)</td>
<td>2.0 $\times 10^{-3}$</td>
</tr>
<tr>
<td>291.2</td>
<td>1.70 $\times 10^{-3}$ (T; Ref. 61)</td>
<td>2.2 $\times 10^{-3}$</td>
</tr>
<tr>
<td>293.0</td>
<td>4.43 $\times 10^{-3}$ (D; Ref. 58)</td>
<td>2.4 $\times 10^{-3}$</td>
</tr>
<tr>
<td>293.2</td>
<td>2.30 $\times 10^{-3}$ (R; Ref. 13), 2.35 $\times 10^{-3}$ (R; Ref. 19), 2.30 $\times 10^{-3}$ (R; Ref. 47)</td>
<td>2.4 $\times 10^{-3}$</td>
</tr>
<tr>
<td>295.2</td>
<td>2.68 $\times 10^{-3}$ (T; Ref. 63)</td>
<td>2.6 $\times 10^{-3}$</td>
</tr>
<tr>
<td>298.2</td>
<td>2.78 $\times 10^{-3}$ (R; Ref. 21), 5.04 $\times 10^{-3}$ (D; Ref. 21), 2.86 $\times 10^{-3}$ (R; Ref. 22), 2.80 $\times 10^{-3}$ (R; Ref. 27), 2.92 $\times 10^{-3}$ (R; Ref. 29), 2.40 $\times 10^{-3}$ (T; Ref. 30), 2.30 $\times 10^{-3}$ (T; Ref. 43), 2.77 $\times 10^{-3}$ (R; Ref. 45), 3.06 $\times 10^{-3}$ (T; Ref. 58), 4.70 $\times 10^{-3}$ (D; Ref. 60)</td>
<td>2.8 $\times 10^{-3}$</td>
</tr>
<tr>
<td>302.9</td>
<td>4.69 $\times 10^{-3}$ (D; Ref. 58)</td>
<td>3.2 $\times 10^{-3}$</td>
</tr>
<tr>
<td>303.0</td>
<td>7.39 $\times 10^{-2}$ (T; Ref. 7)</td>
<td>3.2 $\times 10^{-3}$</td>
</tr>
</tbody>
</table>
Components:
(1) Toluene, C_7H_8, [108-88-3]
(2) Water, H_2O, [7732-18-5]

Original Measurements:

Variables:
Temperature: 99.4 °C–200.4 °C
Pressure: 1.53–23.63 bar

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

Experimental Data
Solubility of toluene in water

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

Solubility of water in toluene

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

Auxiliary Information

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

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

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

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

FIG. 4. Recommended and tentative solubility data for water (2) in toluene (1).
<table>
<thead>
<tr>
<th>Variables:</th>
<th>One temperature: 25 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Prepared By:</td>
<td>A. Maczynski and Z. Maczynska</td>
</tr>
</tbody>
</table>

### Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.053 g (1)/100 g sln. The corresponding mole fraction, $x_1$, calculated by the compilers is 1.04 $\times 10^{-4}$.

#### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

(1) Eastman Kodak Co. best grade; washed successively with concentrated sulfuric acid, water, and dilute sodium hydroxide; dried, and distilled; b.p. 110.4 °C.

(2) Not specified.

**Estimated Error:**

Not specified.
The solubility of toluene in water was reported to be 1.68 $\times 10^{-2}$ mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass percent and mole fraction, $x_1$, solubilities, calculated by the compiler, are 0.155 g(1)/100 g sln and 3.04 $\times 10^{-4}$, respectively.

Auxiliary Information

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

Source and Purity of Materials:
(1) $^{14}$C-labeled toluene: New England Nuclear, used without further purification.
(2) Distilled.

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

Source and Purity of Materials:

Experimental Data

The solubility of water in toluene at 303 K was reported to be 0.0273 g(2)/100 g sln. The corresponding mole fraction, $x_1$, value calculated by compiler is 0.0739.

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; purified; purity not specified.
(2) Distilled.
**Components:**
(1) Toluene; C\(_7\)H\(_8\); [108-88-3]
(2) Water; H\(_2\)O; [7732-18-5]

**Variables:**
Temperature: 10.0 °C and 20.0 °C

**Prepared By:**
A. Skrzecz, I. Owczarek, and K. Blanje

---

### Experimental Data

**Solubility of toluene in water**

<table>
<thead>
<tr>
<th>°C</th>
<th>(10^3) mol (1)/L sln</th>
<th>(10^2) g (1)/100 g sln (compilers)</th>
<th>(10^3) (x_1) (compilers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>6.21</td>
<td>5.72</td>
<td>1.119</td>
</tr>
<tr>
<td>20.0</td>
<td>6.37</td>
<td>5.87</td>
<td>1.149</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

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

**Source and Purity of Materials:**
(1) Fluka, puriss grade, 99.9%; used as received.
(2) Triple distilled.

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

**References:**

---

### Experimental Data

**Solubility of water in toluene**

<table>
<thead>
<tr>
<th>°C</th>
<th>(x_{1}) (1)/100 g sln (compilers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>6.69 (\times 10^{-3})</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

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

**Source and Purity of Materials:**
(1) Fluka, puriss grade, 99.9%; used as received.
(2) Triple distilled.

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

**References:**
Components: Original Measurements:
(1) Toluene; C\textsubscript{7}H\textsubscript{8}; [108-88-3]
(2) Water; H\textsubscript{2}O; [7732-18-5]


Variables: Prepared By:
Temperature: 0.4 °C– 45.3 °C G. T. Hefter

Experimental Data

Solubility of toluene in water

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^4 \cdot x_1 ) (compiler)</th>
<th>g (1/100 g sln)\textsuperscript{a} (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>1.29</td>
<td>0.0658</td>
</tr>
<tr>
<td>3.6</td>
<td>1.26</td>
<td>0.0646</td>
</tr>
<tr>
<td>10.0</td>
<td>1.23</td>
<td>0.0628</td>
</tr>
<tr>
<td>11.2</td>
<td>1.22</td>
<td>0.0624</td>
</tr>
<tr>
<td>14.9</td>
<td>1.22</td>
<td>0.0623</td>
</tr>
<tr>
<td>15.9</td>
<td>1.21</td>
<td>0.0621</td>
</tr>
<tr>
<td>20.0</td>
<td>1.23\textsuperscript{b}</td>
<td>0.0627\textsuperscript{b}</td>
</tr>
<tr>
<td>25.6</td>
<td>1.22</td>
<td>0.0625</td>
</tr>
<tr>
<td>30.0</td>
<td>1.25</td>
<td>0.0640</td>
</tr>
<tr>
<td>30.2</td>
<td>1.28</td>
<td>0.0642</td>
</tr>
<tr>
<td>35.2</td>
<td>1.38</td>
<td>0.0657</td>
</tr>
<tr>
<td>42.8</td>
<td>1.37</td>
<td>0.0701</td>
</tr>
<tr>
<td>45.3</td>
<td>1.40</td>
<td>0.0717</td>
</tr>
</tbody>
</table>

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

\textsuperscript{b}Given in the original paper as 0.627 g(1)/L sln.

Auxiliary Information

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

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

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

Components: Original Measurements:
(1) Toluene; C\textsubscript{7}H\textsubscript{8}; [108-88-3]
(2) Water; H\textsubscript{2}O; [7732-18-5]


Variables: Prepared By:
One temperature: 25.0 °C (298.2 K) G. T. Hefter

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.04 mL (1/100 mL). The solubility of (1) in 40.0% (w/w) aqueous sodium xylene sulfonate solution was also reported to be 1.20 mL (1/100 mL) sulfonate sln.

Auxiliary Information

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

Source and Purity of Materials:
(1) Highest grade commercial sample available; no other details given.
(2) Distilled.

Estimated Error:
Not specified.
**Experimental Data**

Solubility of toluene in water

<table>
<thead>
<tr>
<th>T/°C</th>
<th>$10^4$·$x_1^a$ (g/100 g sln)</th>
<th>$g(1/100 \text{ g sln})^a$ (computer)</th>
<th>mol (1/L sln)</th>
<th>P/bar$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.07</td>
<td>0.0547</td>
<td>0.00595</td>
<td>1</td>
</tr>
<tr>
<td>45</td>
<td>1.41</td>
<td>0.0722</td>
<td>0.00785</td>
<td>1</td>
</tr>
<tr>
<td>55</td>
<td>1.68</td>
<td>0.086</td>
<td>0.0094</td>
<td>1</td>
</tr>
<tr>
<td>45</td>
<td>2.17</td>
<td>0.111</td>
<td>0.0121</td>
<td>1000</td>
</tr>
<tr>
<td>55</td>
<td>2.37</td>
<td>0.121</td>
<td>0.0131</td>
<td>1000</td>
</tr>
</tbody>
</table>

$^a$Assuming a solution density of 1.00 kg/L at all temperatures.

$^b$1 bar = 0.1 MPa exactly.

Data at other pressures are presented in graphical form. Data are also presented for the solubility of H2O in aqueous solutions of AgNO₃ and KNO₃ at various temperatures and pressures.

**Auxiliary Information**

- **Source and Purity of Materials:**
  - (1) Not specified.
  - (2) Distilled, air-free.
- **Estimated Error:**
  - Not specified.

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

---

**Experimental Data**

Solubility of water in toluene

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/MPa</th>
<th>$g(1/100 \text{ g sln})^a$ (computer)</th>
<th>$10^4$·$x_2^a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>340.6</td>
<td>6.80</td>
<td>0.093</td>
<td>0.183 ± 0.005</td>
</tr>
<tr>
<td>384.1</td>
<td>6.80</td>
<td>0.184</td>
<td>0.360 ± 0.008</td>
</tr>
<tr>
<td>403.2</td>
<td>6.80</td>
<td>0.269</td>
<td>0.527 ± 0.010</td>
</tr>
<tr>
<td>417.2</td>
<td>6.80</td>
<td>0.353</td>
<td>0.693 ± 0.014</td>
</tr>
<tr>
<td>445.0</td>
<td>6.80</td>
<td>0.600</td>
<td>1.18 ± 0.02</td>
</tr>
<tr>
<td>485.2</td>
<td>6.80</td>
<td>1.36</td>
<td>2.68 ± 0.05</td>
</tr>
<tr>
<td>518.0</td>
<td>6.80</td>
<td>2.74</td>
<td>5.47 ± 0.11</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- **Source and Purity of Materials:**
  - (1) Aldrich Chemicals Co.; HPLC grade purity 99.8 mass%.
  - (2) Aldrich Chemicals Co.; HPLC grade.
- **Estimated Error:**
  - Temperature: ±0.2 K (precision of measurements), ±1 K (reproducibility).
  - Pressure: ±0.001 MPa.
  - Solubility: as above.

**References:**

Components:
(1) Toluene; C\textsubscript{7}H\textsubscript{8}; [108-88-3]
(2) Water; H\textsubscript{2}O; [7732-18-5]

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

Prepared By:
G. T. Hefter

Experimental Data

Solubility of toluene in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10\textsuperscript{9} x\textsubscript{1} (compiler)</th>
<th>g(1)/100 g sln\textsuperscript{*}</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.5</td>
<td>1.20</td>
<td>0.0612 ± 0.0010</td>
</tr>
<tr>
<td>6.3</td>
<td>1.18</td>
<td>0.0604 ± 0.0014</td>
</tr>
<tr>
<td>7.1</td>
<td>1.15</td>
<td>0.0586 ± 0.0018</td>
</tr>
<tr>
<td>9.0</td>
<td>1.15</td>
<td>0.0587 ± 0.0011</td>
</tr>
<tr>
<td>11.8</td>
<td>1.12</td>
<td>0.0573 ± 0.0014</td>
</tr>
<tr>
<td>12.1</td>
<td>1.13</td>
<td>0.0575 ± 0.0012</td>
</tr>
<tr>
<td>15.1</td>
<td>1.11</td>
<td>0.0569 ± 0.0013</td>
</tr>
<tr>
<td>17.9</td>
<td>1.13</td>
<td>0.0577 ± 0.0013</td>
</tr>
<tr>
<td>20.1</td>
<td>1.11</td>
<td>0.0566 ± 0.0011</td>
</tr>
</tbody>
</table>

\textsuperscript{*}Errors given as standard deviation.

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

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

Auxiliary Information

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

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

Components:
(1) Toluene; C\textsubscript{7}H\textsubscript{8}; [108-88-3]
(2) Water; H\textsubscript{2}O; [7732-18-5]

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Data

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

The corresponding mass percent and mole fraction, x\textsubscript{2}, calculated by the compiler are 0.046 g(2)/100 g sln and 0.0023.

Auxiliary Information

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

Estimated Error:
Temperature: ±0.01 °C.

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

Source and Purity of Materials:
(1) Fluka, puriss grade, purity >99.5%; used as received.
(2) Triply distilled.

Estimated Error:
Temperature: ±0.2 °C.
Solubility: 1% (reproducibility of measurements).
Components: (1) Toluene; C₇H₈; [108-88-3]
(2) Water; H₂O; [7732-18-5]

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

Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>T/°C</th>
<th>P/bar</th>
<th>g(1/100 g sln (compilers))</th>
<th>10² x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>25</td>
<td>1.21</td>
<td>0.238±0.017</td>
</tr>
<tr>
<td>250</td>
<td>58</td>
<td>3.49</td>
<td>0.703±0.095</td>
</tr>
<tr>
<td>250</td>
<td>172 a</td>
<td>3.55</td>
<td>0.714±0.029</td>
</tr>
<tr>
<td>275</td>
<td>86</td>
<td>6.27</td>
<td>1.29±0.06</td>
</tr>
<tr>
<td>275</td>
<td>172 a</td>
<td>6.27</td>
<td>1.29±0.04</td>
</tr>
</tbody>
</table>

Solubility of water in toluene

<table>
<thead>
<tr>
<th>T/°C</th>
<th>P/bar</th>
<th>g(2/100 g sln (compilers))</th>
<th>x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>25</td>
<td>5.58</td>
<td>0.232±0.031</td>
</tr>
<tr>
<td>250</td>
<td>58</td>
<td>10.86</td>
<td>0.384±0.032</td>
</tr>
<tr>
<td>250</td>
<td>172 a</td>
<td>8.97</td>
<td>0.335±0.013</td>
</tr>
<tr>
<td>275</td>
<td>86</td>
<td>20.52</td>
<td>0.569±0.015</td>
</tr>
<tr>
<td>275</td>
<td>172 a</td>
<td>13.94</td>
<td>0.453±0.015</td>
</tr>
</tbody>
</table>

*Pressure above the three-phase pressure.

Auxiliary Information

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

Source and Purity of Materials:
(1) Aldrich Chemical Co.; HPLC grade reagent; purity >99.8%; used as received.
(2) Aldrich Chemical Co.; HPLC grade water.

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

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The continuous flow equilibrium apparatus for mutual solubility measurements, Chen and Wagner was used. Samples were collected in 25 mL vials and 60 and 120 mL bottles containing dehydrated ethanol or 2,2,4-trimethylpentane as a solvent. Details of the standard preparation, calibration, and sampling procedures were described in the paper. A Hewlett-Packard 5880A gas chromatograph equipped with Porapak or Glass Chrom 254 columns and a thermal conductivity detector were used for analysis. Reported solubilities are the average of 6–13 replicate determinations.

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

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

References:
Components:
(1) Toluene; C\textsubscript{7}H\textsubscript{8} [108-88-3]
(2) Water; H\textsubscript{2}O. [7732-18-5]

Original Measurements:

Variables:
One temperature; 21 °C

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

---

### Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>g (1)/100 g sln</th>
<th>x\textsubscript{1} (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>0.0479±0.0086</td>
<td>9.36·10^{-5}</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; A.R. reagent; used as received.
(2) Distilled water.

Estimated Error:
Temperature: ± 1 °C.
Solubility: ± 0.01.

---

Components:
(1) Toluene; C\textsubscript{7}H\textsubscript{8} [108-88-3]
(2) Water; H\textsubscript{2}O. [7732-18-5]

Original Measurements:

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

Prepared By:
A. Maczynski and Z. Maczynska

### Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>x\textsubscript{1} (compiler)</th>
<th>g (1)/100 g sln</th>
<th>P/MPa (compiler)</th>
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<td>0.0313</td>
<td>14.2</td>
<td>17.2</td>
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<tr>
<td>300</td>
<td>0.0311</td>
<td>14.1</td>
<td>25.3</td>
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<tr>
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<tr>
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<td>19.0</td>
<td>250</td>
</tr>
<tr>
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<td>0.0411</td>
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<tr>
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<tr>
<td>310</td>
<td>0.0590</td>
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<tr>
<td>310</td>
<td>0.0759</td>
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<td>17.7</td>
</tr>
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<td>310</td>
<td>0.0882</td>
<td>33.1</td>
<td>18.2</td>
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<td>310</td>
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<td>36.3</td>
<td>18.2</td>
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<td>310</td>
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<tr>
<td>310</td>
<td>0.1452</td>
<td>46.5</td>
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<td>310</td>
<td>0.1002</td>
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<td>260</td>
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<td>310</td>
<td>0.0882</td>
<td>33.1</td>
<td>260</td>
</tr>
<tr>
<td>310</td>
<td>0.0759</td>
<td>29.6</td>
<td>275</td>
</tr>
<tr>
<td>310</td>
<td>0.0665</td>
<td>26.7</td>
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<td>0.0578</td>
<td>23.8</td>
<td>325</td>
</tr>
<tr>
<td>310</td>
<td>0.0452</td>
<td>19.5</td>
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</tr>
<tr>
<td>310</td>
<td>0.0411</td>
<td>11.0</td>
<td>455</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

Source and Purity of Materials:
(1) Phillips reagent grade; better than 99.8%; used as received.
(2) Distilled and degased.

Estimated Error:
Temperature: ± 0.02 °C.
Pressure: ± 2 atm.
### Components:

1. **Toluene**; C\textsubscript{7}H\textsubscript{8}; [108-88-3]
2. **Water**; H\textsubscript{2}O; [7732-18-5]

### Original Measurements:


### Variables:

- **Temperature**: 273.65 K–328.15 K

#### Experimental Data

**Solubility of toluene in water**

<table>
<thead>
<tr>
<th>T/K</th>
<th>10\textsuperscript{3} mol/L in sln</th>
<th>10\textsuperscript{4} g(1)/100 g sln (compiler)</th>
<th>10\textsuperscript{4} x\textsubscript{1}</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.65</td>
<td>6.11</td>
<td>5.62</td>
<td>1.10</td>
</tr>
<tr>
<td>278.15</td>
<td>5.99</td>
<td>5.52</td>
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<td>288.15</td>
<td>5.88</td>
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<td>1.06</td>
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<td>298.15</td>
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<td>1.09</td>
</tr>
<tr>
<td>308.25</td>
<td>6.40</td>
<td>5.93</td>
<td>1.16</td>
</tr>
<tr>
<td>318.15</td>
<td>6.86</td>
<td>6.39</td>
<td>1.25</td>
</tr>
<tr>
<td>328.15</td>
<td>7.64</td>
<td>7.16</td>
<td>1.40</td>
</tr>
</tbody>
</table>

#### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Temperature: ±0.01 K.

### Components:

1. **Water**; H\textsubscript{2}O; [7732-18-5]

### Original Measurements:


### Variables:

- **Temperature**: 0 °C–50 °C

#### Experimental Data

**Solubility of water in toluene**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10\textsuperscript{3} x\textsubscript{2} (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.382</td>
<td>0.02704</td>
</tr>
<tr>
<td>10</td>
<td>1.61</td>
<td>0.0316</td>
</tr>
<tr>
<td>20</td>
<td>2.35</td>
<td>0.0460</td>
</tr>
<tr>
<td>30</td>
<td>3.14</td>
<td>0.0615</td>
</tr>
<tr>
<td>40</td>
<td>3.82</td>
<td>0.0750</td>
</tr>
<tr>
<td>50</td>
<td>4.92</td>
<td>0.0965</td>
</tr>
</tbody>
</table>

#### Auxiliary Information

**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.

**Estimated Error:**

Not specified.
Components: 
(1) Toluene, C₇H₈, [108-88-3] 
(2) Water, H₂O, [7732-18-5]

Original Measurements: 

Variables: 
One temperature: 16 °C

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

Experimental Data

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

The corresponding mole fraction, x₁, calculated by the compilers is 9.2 • 10⁻⁵.

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components: 
(1) Toluene, C₇H₈, [108-88-3] 
(2) Water, H₂O, [7732-18-5]

Original Measurements: 

Variables: 
Temperature: 15°C–30 °C

Prepared By: 
A. Maczynski and Z. Maczynska

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁻³x₂ (compiler)</th>
<th>ρ(2)/100 g sln (compiler)</th>
<th>mol (2)/L sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>2.11</td>
<td>0.0413</td>
<td>0.0200±0.0006</td>
</tr>
<tr>
<td>25</td>
<td>2.78</td>
<td>0.0545</td>
<td>0.0261±0.0004</td>
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<tr>
<td>30</td>
<td>3.14</td>
<td>0.0615</td>
<td>0.0293±0.0004</td>
</tr>
</tbody>
</table>

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

Auxiliary Information

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

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

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

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

Estimated Error:
Solubility: as indicated above (type of error not specified).
Experimental Data

The solubility of water in toluene at 25 °C was reported to be 0.0268 mol L⁻¹ sln.

The corresponding mass percent and mole fraction, x₂, calculated by the compilers are 0.0560 g/100 g sln and 2.86 \times 10⁻³.

The assumption that 1 L sln = 863 g sln was used in the calculation.

Auxiliary Information

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

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

Estimated Error:
Temperature: ±0.05 °C.

References:

Experimental Data

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

The corresponding mass percent and mole fraction, x₁, calculated by the compilers are 0.057 g/100 g sln and 1.12 \times 10⁻⁴.

Auxiliary Information

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

Source and Purity of Materials:
(1) Baker’s CP analyzed grade; distilled; b.p. 110.74 ±0.02 °C.
(2) Distilled.

Estimated Error:
Solubility: 2.0% (from values of duplicate determinations).
### Components:

- **Toluene**: C₇H₈, 108-88-3
- **Water**: H₂O, 7732-18-5

### Original Measurements:


### Variables:

- **Temperature**: 90 °C–224 °C
- **Pressure**: 10.5 MPa–28.1 MPa

### Experimental Data

#### Solubility of toluene in water

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10³ x₁ (compiler)</th>
<th>g(1)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.42</td>
</tr>
<tr>
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<tr>
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<tr>
<td>224</td>
<td>10.336</td>
<td>5.072</td>
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</table>

#### Mutual solubility of toluene in water

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/MPa</th>
<th>g(1)/100 g sln (compilers)</th>
<th>x₁</th>
</tr>
</thead>
<tbody>
<tr>
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<td>15.3</td>
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<tr>
<td>583.2</td>
<td>18.3</td>
<td>0.201</td>
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<td>20.4</td>
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<td>22.2</td>
<td>0.205</td>
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<td>25.2</td>
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<tr>
<td>28.1</td>
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<td>0.044±0.0011</td>
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#### Mutual solubility of water in toluene

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/MPa</th>
<th>g(2)/100 g sln (compilers)</th>
<th>x₂</th>
</tr>
</thead>
<tbody>
<tr>
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<td>56.9</td>
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<tr>
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</tr>
<tr>
<td>22.2</td>
<td>41.2</td>
<td>0.782±0.0080</td>
<td></td>
</tr>
<tr>
<td>25.2</td>
<td>38.1</td>
<td>0.759±0.0055</td>
<td></td>
</tr>
<tr>
<td>28.1</td>
<td>36.4</td>
<td>0.745±0.0076</td>
<td></td>
</tr>
</tbody>
</table>

### Auxiliary Information

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

**Source and Purity of Materials:**
(1) Wako Pure Chem. Ind.; purity >99.5 mole % by glc; used as received.
(2) Distilled water was purified by MilliQ Lab. (Millipore Co.) equipment

**Estimated Error:**
Temperature: ±1 K.
Pressure: ±0.1 MPa.

**References:**
Components: Original Measurements:
(1) Toluene: C₇H₈; [108-88-3]
(2) Water: H₂O; [7732-18-5]

Variables: Prepared By:
One temperature: 25 °C
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in toluene was reported to be 0.026 mol/L sln.
The corresponding mass percent and mol fraction, x₂, calculated by the compilers are 0.054 g(2)/100 g sln and 2.8 \times 10^{-3}. The assumption that 1 L sln=862 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The water determination was carried out according to Johansson’s modification of the Karl Fischer titration in Hardy et al.¹ and Johansson.²

Source and Purity of Materials:
(1) Kebo, purity 99.0%; used as received.
(2) Not specified.

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

References:

Components: Original Measurements:
(1) Toluene: C₇H₈; [108-88-3]
(2) Water: H₂O; [7732-18-5]
A. Jäger, Brennst.-Chem. 4, 259 (1923).

Variables: Prepared By:
Temperature: 100 °C–300 °C
A. Maczynski

Experimental Data

Solubility of toluene in water

<table>
<thead>
<tr>
<th>°C</th>
<th>mL (1/100 mL (2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>0.2</td>
</tr>
<tr>
<td>200</td>
<td>0.7</td>
</tr>
<tr>
<td>250</td>
<td>2.8</td>
</tr>
<tr>
<td>300</td>
<td>13.0</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined in sealed glass tubes.

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

Estimated Error:
Not specified.
**Components:**

(1) Toluene; C\textsubscript{7}H\textsubscript{8}; [108-88-3]
(2) Water; H\textsubscript{2}O; [7732-18-5]

**Original Measurements:**


**Variables:**

One temperature: 25 °C

**Prepared By:**

A. Maczynski and Z. Maczynska

---

### Experimental Data

**Solubility of water in toluene**

<table>
<thead>
<tr>
<th>°C</th>
<th>( \times 10^2 \text{ mol(2)/L sln} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>4.0</td>
</tr>
<tr>
<td>30</td>
<td>4.8</td>
</tr>
<tr>
<td>35</td>
<td>5.9</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

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

**References:**

**Components:**

1. Toluene; C7H8; 108-88-3
2. Water; H2O; 7732-18-5

**Original Measurements:**


**Variables:**

One temperature: 25.00 °C

**Prepared By:**

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

**Experimental Data**

**Solubility of toluene in water**

<table>
<thead>
<tr>
<th>°C</th>
<th>mol (1/L sln)</th>
<th>g(1)/100 g sln</th>
<th>x1</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.00</td>
<td>(6.29±0.03) × 10^-3</td>
<td>0.05 g(1)/100 g sln</td>
<td>(1.13±0.01) × 10^-4</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Temperature: ±0.01 °C.
Solubility: ±0.01 g/L (standard deviation of the mean).

**References:**

The solubility of toluene in water at 25 °C was reported to be 0.65 g(1)/L sln. The corresponding mass percent and mole fraction, $x_1$, calculated by the compilers are 0.065 g(1)/100 g sln and 1.27 $\times 10^{-4}$. The compiler's calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

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

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

Estimated Error: Solubility: ±0.01 g(1)/L sln (standard deviation from 6 determinations).
Components: (1) Toluene; C₇H₈; [108-88-3](2) Water; H₂O; [7732-18-5]

Variables: One temperature: 25 °C

Prepared By: A. Maczynski

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.220 mg (1)/mL sln. The corresponding mass percent and mole fraction, x₁, calculated by the compiler are 0.022 g/(1/100 g sln) and 4.3 • 10⁻⁵. The compiler's calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

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

Estimated Error: Temperature: ±1 °C.


Source and Purity of Materials:
(1) Described in Ref. 1. (2) Distilled.

Components: (1) Toluene; C₇H₈; [108-88-3](2) Water; H₂O; [7732-18-5]

Variables: One temperature: 25 °C

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

Experimental Data

Solubility of toluene in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>g (1)/100 g sln x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.052±0.002 1.02 • 10⁻⁴</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure: The radiometric method was used. The radiotracer ⁶⁰Co(PDC)₃ was first dissolved in component (1) before pure water was added. Both of the liquids were placed in a 1000 mL separation funnel. The mixture was shaken for 5 min and allowed to separate for next 30 min. Concentration was calculated from activity measurements by a NaI(Tl) scintillation detector.


Source and Purity of Materials: (1) E. Merck; purity not specified. (2) Demineralized and degassed.

Estimated Error: Solubility: as above (standard deviation of mean).
### Components:
1. Toluene; C\(_7\)H\(_8\); [108-88-3]
2. Water; H\(_2\)O; [7732-18-5]

### Variables:
- **Temperature: 5.0 °C–45.0 °C**

### Prepared By:
- A. Skrzecz, I. Owczarek, and K. Blanej

### Experimental Data

#### Solubility of toluene in water

<table>
<thead>
<tr>
<th>(t/°C)</th>
<th>(g/100\ \text{g sln})</th>
<th>(10^3\cdot x_1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.0</td>
<td>540±29</td>
<td>5.42</td>
</tr>
<tr>
<td>15.0</td>
<td>516±16</td>
<td>5.16</td>
</tr>
<tr>
<td>25.0</td>
<td>519±5.0</td>
<td>5.21</td>
</tr>
<tr>
<td>35.0</td>
<td>555±30</td>
<td>5.57</td>
</tr>
<tr>
<td>45.0</td>
<td>632±21</td>
<td>6.39</td>
</tr>
</tbody>
</table>

### Auxiliary Information

#### Method/Apparatus/Procedure:
The analytical method was used. Saturated solutions were prepared by adding an excess of (1) to a 125 mL or 250 mL Erlenmeyer flask containing (2). The flask was shaken and magnetically stirred for 24 h, and next allowed to settle in a constant temperature bath (Neslab Model RTE-8) for at least 48 h. A Hewlett-Packard Model 5750 equipped with a hydrogen flame ionization detector was used for analysis of hexane extracts. All experimental points are the mean of more than 9 determinations.

#### Source and Purity of Materials:
- (1) Caledon Laboratories, Georgetown, Ontario; HPLC grade; used as received.
- (2) Not specified.

#### Estimated Error:
- Temperature: ±0.5 °C
- Solubility: as above.

---

### Components:
2. Water; H\(_2\)O; [7732-18-5]

### Variables:
- One temperature: 25 °C

### Prepared By:
- M. C. Hauliat-Pirson

### Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.5195 g/100 g sln. The corresponding mass percent and mole fraction, \(x_1\), calculated by the compiler are 0.05195 g(1)/100 g sln and 1.015 \(\times\) 10\(^{-4}\). The compiler’s calculations assume a solution density of 1.00 g/mL.

### Auxiliary Information

#### Source and Purity of Materials:
- (1) Phillips Petroleum Co.; research grade; 99.9+%; used as received.
- (2) Not specified.

#### Estimated Error:
- Temperature: ±0.1 °C.
- Solubility: ±0.0096 g(1)/L.
Experimental Data

The solubility of toluene in water at 25 °C was reported to be 0.0538 g/(100 g sln). The corresponding mole fraction, $x_1$, calculated by the compilers is 1.05 $\times$ 10^{-4}.

Auxiliary Information

Method/Apparatus/Procedure:
The saturated solutions of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer.

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

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 0.0017 (standard deviation of mean).
Components:
(1) Toluene; C7H8; [108-88-3]
(2) Water; H2O; [7732-18-5]

Original Measurements:

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

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

Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>T/K</th>
<th>P/bar</th>
<th>g(1)/100 g sln compilers</th>
<th>10^3 * x_1</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.0</td>
<td>50</td>
<td>0.0547</td>
<td>0.107±0.002</td>
</tr>
<tr>
<td>323.0</td>
<td>50</td>
<td>0.0639</td>
<td>0.125±0.004</td>
</tr>
<tr>
<td>373.0</td>
<td>50</td>
<td>0.138</td>
<td>0.27±0.01</td>
</tr>
<tr>
<td>423.0</td>
<td>50</td>
<td>0.337</td>
<td>0.66±0.03</td>
</tr>
<tr>
<td>473.0</td>
<td>50</td>
<td>0.964</td>
<td>1.9±0.1</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The dynamic method described in Miller and Hawthorne1 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:

Components:
(1) Toluene; C7H8; [108-88-3]
(2) Water; H2O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Data
The solubility of toluene in water at 25 °C was reported to be 0.00582 mol (1)/1000 g (2).
The corresponding mass percent and mole fraction, x_1, calculated by compilers are 0.0536 g(1)/100 g sln and x_1 = 1.05·10^{-4}.
The compiler’s calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

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

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

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.5% (mean of large numbers of determinations).
Components:
(1) Toluene; C₇H₈; [108-88-3]
(2) Water; H₂O; [7732-18-5]

Variables:
One temperature: 25.0 °C

Experimental Data
Solubility of water in toluene

<table>
<thead>
<tr>
<th>T/°C</th>
<th>x₁</th>
<th>x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>0.045</td>
<td>0.0023</td>
</tr>
</tbody>
</table>

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 Porapak Q column.

Source and Purity of Materials:
(1) Aldrich Chemical Co; glc grade; purity 99.9 mass %; used as received.
(2) Deionized water.

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

Estimated Error:
Temperature: ±0.1 °C.

Components:
(1) Toluene; C₇H₈; [108-88-3]
(2) Water; H₂O; [7732-18-5]

Variables:
Temperature: 278.16 K–318.46 K

Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>T/K</th>
<th>x₁</th>
<th>g(1)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>278.16</td>
<td>0.1243</td>
<td>0.06355±0.0017</td>
</tr>
<tr>
<td>283.06</td>
<td>0.1236</td>
<td>0.06324±0.0016</td>
</tr>
<tr>
<td>293.06</td>
<td>0.1292</td>
<td>0.06606±0.0018</td>
</tr>
<tr>
<td>298.16</td>
<td>0.1232</td>
<td>0.06299±0.0013</td>
</tr>
<tr>
<td>308.26</td>
<td>0.1314</td>
<td>0.06721±0.0011</td>
</tr>
<tr>
<td>318.46</td>
<td>0.1313</td>
<td>0.06717±0.0020</td>
</tr>
</tbody>
</table>

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

Source and Purity of Materials:
(1) Fisher Scientific Co., Chromatoquality; 99+ mole %; used as received.
(2) Laboratory distilled water.

Prepared By:
M. C. Haunlat-Pirson

Estimated Error:
Solubility: standard deviation, from at least 15 measurements are given above.
Components:
(1) Toluene; C₇H₈; [108-88-3]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
Temperature: 0 °C–25 °C
Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁶ x₁ (compiler)</th>
<th>g(1)/100 g sln (compiler)</th>
<th>mg (1)/kg(2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>1.42</td>
<td>0.0724</td>
<td>72.4</td>
</tr>
<tr>
<td>25°</td>
<td>1.12</td>
<td>0.0573</td>
<td>57.3</td>
</tr>
</tbody>
</table>

Solubility of water in toluene

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁵ x₂ (compiler)</th>
<th>g(2)/100 g sln (compiler)</th>
<th>mg (2)/kg(1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>1.17</td>
<td>0.0228</td>
<td>22.8</td>
</tr>
<tr>
<td>25°</td>
<td>2.77</td>
<td>0.0545</td>
<td>54.5</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

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

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

Source and Purity of Materials:
(1) Matheson, Coleman and Bell, spectroquality grade reagent; shaken three times with distilled water.
(2) Distilled.

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

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A. MACZYŃSKI AND D. G. SHAW
### Components:
- Toluene; C\textsubscript{7}H\textsubscript{8}; 108-88-3
- Water; H\textsubscript{2}O; 7732-18-5

### Original Measurements:

### Variables:
- Temperature: 10 °C– 50 °C
- One temperature: 25 °C

### Prepared By:
- A. Maczynski and Z. Maczynska
- G. T. Hefter

### Experimental Data

#### Solubility of water in toluene

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^3 \times x_2 ) (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.71</td>
<td>0.0335</td>
</tr>
<tr>
<td>20</td>
<td>2.30</td>
<td>0.0450</td>
</tr>
<tr>
<td>30</td>
<td>3.06</td>
<td>0.0600</td>
</tr>
<tr>
<td>40</td>
<td>3.74</td>
<td>0.0735</td>
</tr>
<tr>
<td>50</td>
<td>4.85</td>
<td>0.0953</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

- Temperature: ± 0.1 °C.
- Solubility: ± 6.1 μg/g (standard deviation for 6 determinations).

### Source and Purity of Materials:

1. Burdick & Jackson; purified by triple distillation in glass.
2. Doubly distilled in all-glass apparatus; free of trace organics.

### Estimated Error:

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

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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>108-88-3</td>
</tr>
<tr>
<td>Water</td>
<td>7732-18-5</td>
</tr>
</tbody>
</table>

### Original Measurements:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>108-88-3</td>
</tr>
<tr>
<td>Water</td>
<td>7732-18-5</td>
</tr>
</tbody>
</table>

### Variables:

One temperature: 25 °C

### Prepared By:


### Experimental Data

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

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

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

**References:**


### Components:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS Number</th>
</tr>
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<tbody>
<tr>
<td>Toluene</td>
<td>108-88-3</td>
</tr>
<tr>
<td>Water</td>
<td>7732-18-5</td>
</tr>
</tbody>
</table>

### Original Measurements:

<table>
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<th>Component</th>
<th>CAS Number</th>
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<tbody>
<tr>
<td>Toluene</td>
<td>108-88-3</td>
</tr>
<tr>
<td>Water</td>
<td>7732-18-5</td>
</tr>
</tbody>
</table>

### Variables:

One temperature: 25 °C

### Prepared By:

G. T. Hefter

### Experimental Data

The solubility of toluene in water at 25 °C was reported to be 5.65 × 10⁻³ mol(1)/L sln. Assuming a solution density of 1.00 kg/L this corresponds to a solubility of 0.0521 g(1)/100 g sln, x₁ = 1.02 × 10⁻⁶, calculated by the compiler.

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

(1) Analytical reagent grade source not stated, used without further purification. (2) Deionized and redistilled; no further details given.

**Estimated Error:**

Not specified.

**References:**

### Experimental Data

#### The solubility of toluene in water

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<th>$10^3 \cdot x_1$ (g/mol/L sln)</th>
<th>$g(1)/100$ g sln (pure)</th>
<th>$10^3 \cdot mol(1)/L$ sln</th>
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<tbody>
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<tr>
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<td>0.0584</td>
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</table>

*Assuming the solution density to be that of pure water at the same temperature.*

### Auxiliary Information

**Method/Apparatus/Procedure:**
The apparatus was similar to an earlier design (Sanemasa *et al.*[2]) and was described in detail in the paper. Liquid 1 (toluene) and redistilled liquid 2 were placed in a vessel and a thermostatted funnel, respectively. The solution vapor, generated by bubbling air through the liquid solute, was transferred to the flask via a circulating pump. The concentration of the solute was determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

**Source and Purity of Materials:**
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 99.0%, used without further purification.
(2) Redistilled; no further details given.

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

**References:**

### Experimental Data

#### Solubility of toluene in water

<table>
<thead>
<tr>
<th>t°C</th>
<th>$10^3 \cdot x_1$ (g/mol/L sln)</th>
<th>$g(1)/100$ g sln (pure)</th>
<th>$g(1)/L$ sln</th>
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<tr>
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<td>45</td>
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*Assuming the solution density to be that of pure water at the same temperature.*

### Auxiliary Information

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

**Source and Purity of Materials:**
(1) Analytical reagent grade used as purchased.
(2) Redistilled.
Components: Original Measurements:
(1) Toluene: C₇H₈ [108-88-3]
(2) Water: H₂O [7732-18-5]

Variables:
One temperature: 25.0 °C
Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of toluene in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>mol (1/L sln)</th>
<th>g (1/100 g sln (compilers))</th>
<th>s₁ (compilers)</th>
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<td>5.22 10⁻²</td>
<td>1.021 10⁻¹</td>
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</table>

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water and a few drops of toluene were placed in a high pressure optical cell with a Teflon ball for stirring as described in Sawamura et al.¹ The sample was pressurized and shaken in a thermostated water bath for 5 h. The absorbance was measured with a Hitachi Model 340 double-beam spectrophotometer. Details of the apparatus, procedures, and purification were reported in Ref. 1. Solubilities were calculated through the Lambert-Beer’s law with use of the molar extinction coefficients. The ratios of solubilities at high and atmospheric pressures are the average of at least 3 measurements.

References:

Components: Original Measurements:
(1) Toluene: C₇H₈ [108-88-3]
(2) Water: H₂O [7732-18-5]

Variables:
Temperature: 25.00 °C
Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of toluene in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>P/MPa</th>
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<th>s₁/x₁</th>
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<th>10⁴ s₁ (compilers)</th>
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</table>

s₁/x₁ = relation of solubilities at high and normal pressure.

Auxiliary Information

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

References:
### Components:
- Toluene: C₇H₈, [108-88-3]
- Water: H₂O, [7732-18-5]

### Original Measurements:

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

### Prepared By:
- A. Skrzecz, I. Owczarek, and K. Blażej

### Experimental Data

<table>
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<th>T/K</th>
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<td>1.342</td>
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### Auxiliary Information

#### Method/Apparatus/Procedure:
The analytical method was used. Water and a few drops of toluene were placed in a high pressure optical cell with a Teflon ball for stirring as described in Ref. 1. The sample was pressurized and shaken in a thermostatted water bath for a few days. The absorbance was measured at the absorption maximum around 260 nm. Details of the apparatus, procedures, and purification were reported in Sawamura et al.\(^1\,^2\). Solubilities were calculated on the basis of measurements and recommended solubility value at 298.15 K and 0.1 MPa reported in Shaw.\(^3\)

#### Source and Purity of Materials:
1. Nacalai Tesque, Co.; shaken successively with H₂SO₄, Na₂CO₃ aq, H₂O, dried over MgSO₄, distilled; Sawamura et al.\(^1\).
2. Deionized; distilled over trace of KMnO₄; Sawamura et al.\(^2\).

#### Estimated Error:
Temperature: ±0.1 K (compilators).

#### References:
Components: Toluene; C₇H₈; 108-88-3
Water; H₂O; 7732-18-5

Original Measurements:
F. P. Schwarz, Anal. Chem. 52, 10 (1980).

Variables: Prepared By:
One temperature: 23.5 °C M. C. Haulait-Pirson

Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁴ x₁ (compiler)</th>
<th>g(1/100 g sln)</th>
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</thead>
<tbody>
<tr>
<td>23.5</td>
<td>1.31</td>
<td>0.0670 ± 0.0015</td>
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<tr>
<td>23.5</td>
<td>1.29</td>
<td>0.0660 ± 0.0006</td>
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Auxiliary Information

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

Source and Purity of Materials:
(1) 99.9% purity used without further purification.
(2) Distilled.

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

Components: Toluene; C₇H₈; 108-88-3
Water; H₂O; 7732-18-5

Original Measurements:

Variables: Prepared By:
Temperature: 10.0 °C–30.0 °C A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data
Solubility of toluene in water

<table>
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<tr>
<th>t/°C</th>
<th>g(1/100 g sln)</th>
<th>10⁴ x₁ (compiler)</th>
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Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; purity 99.9 mass %; used as received.
(2) Distilled water.

Estimated Error:
Temperature: ±0.5 °C.
Solubility: ±0.5% (average standard deviation).

References:
1F. P. Schwarz, Anal. Chem. 52, 10 (1980).
Components: 
(1) Toluene: C₇H₈; [108-88-3] 
(2) Water: H₂O; [7732-18-5]

Original Measurements:

Variables:
Temperature: 0 °C–90.2 °C

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

Experimental Data
Solubility of toluene in water

<table>
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<tr>
<th>°C</th>
<th>10⁻¹·x₁ (g/100 g sln)</th>
<th>10⁻⁴·x₁ (compilers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.12</td>
<td>2.3</td>
</tr>
<tr>
<td>9.5</td>
<td>0.09</td>
<td>1.8</td>
</tr>
<tr>
<td>19.8</td>
<td>0.08</td>
<td>1.6</td>
</tr>
<tr>
<td>25.0°</td>
<td>0.053</td>
<td>1.0</td>
</tr>
<tr>
<td>29.7</td>
<td>0.08</td>
<td>1.6</td>
</tr>
<tr>
<td>39.6</td>
<td>0.10</td>
<td>2.0</td>
</tr>
<tr>
<td>40.0°</td>
<td>0.06</td>
<td>1.2</td>
</tr>
<tr>
<td>50.0</td>
<td>0.09</td>
<td>1.8</td>
</tr>
<tr>
<td>60.1</td>
<td>0.10</td>
<td>2.0</td>
</tr>
<tr>
<td>70.4</td>
<td>0.09</td>
<td>1.8</td>
</tr>
<tr>
<td>81.0</td>
<td>0.13</td>
<td>2.5</td>
</tr>
<tr>
<td>90.2</td>
<td>0.12</td>
<td>2.3</td>
</tr>
</tbody>
</table>

*Part of ternary solubility measurements.

Solubility of water in toluene

<table>
<thead>
<tr>
<th>°C</th>
<th>10⁻¹·x₂ (g/100 g sln)</th>
<th>10⁻⁴·x₂ (compilers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.042</td>
<td>0.21</td>
</tr>
<tr>
<td>9.5</td>
<td>0.057</td>
<td>0.29</td>
</tr>
<tr>
<td>19.8</td>
<td>0.087</td>
<td>0.44</td>
</tr>
<tr>
<td>25.0°</td>
<td>0.060</td>
<td>0.31</td>
</tr>
<tr>
<td>29.7</td>
<td>0.092</td>
<td>0.47</td>
</tr>
<tr>
<td>39.6</td>
<td>0.110</td>
<td>0.56</td>
</tr>
<tr>
<td>40.0°</td>
<td>0.110</td>
<td>0.56</td>
</tr>
<tr>
<td>50.0</td>
<td>0.140</td>
<td>0.71</td>
</tr>
<tr>
<td>60.1</td>
<td>0.151</td>
<td>0.77</td>
</tr>
<tr>
<td>70.4</td>
<td>0.206</td>
<td>1.04</td>
</tr>
<tr>
<td>81.0</td>
<td>0.247</td>
<td>1.25</td>
</tr>
<tr>
<td>90.2</td>
<td>0.281</td>
<td>1.42</td>
</tr>
</tbody>
</table>

*Part of ternary solubility measurements.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Toluene (1) and water (2) were brought into equilibrium at a given temperature in a thermostat, and samples of each layer were removed by syringe for analysis. To each sample a higher boiling organic compound was added as a standard and the ratio of peaks was measured by gas chromatography, Stephenson et al.¹ ²

Temperature was measured by a calibrated thermometer accurate to 0.1 °C.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; purity >99.9 mass %.
(2) Not stated.

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

References:
Components: Original Measurements:

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water: H₂O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

Variables: Prepared By:

One temperature: 25 °C

A. Maczynski and Z. Maczynska

Experimental Data

The solubility of toluene in water at 25 °C was reported to be 534.8 mg (1)/100 g sln.

The corresponding mass percent and mole fraction, x₁, calculated by the compilers are 0.05348 g (1)/100 g sln and 1.046 • 10⁻⁴.

Auxiliary Information

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

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 4.9 mg (1)/100 g sln (standard deviation of the mean for six replicates).

Source and Purity of Materials:

(1) Aldrich Chemical Co., purity 99.8 mass %; purity >99.8 mass % checked by glc; µ<sup>H</sup> 0.86235; used as received.
(2) Wako Pure Chemical, purity 99.9 mass %, µ<sup>H</sup> 0.99602.

Estimated Error:

Solubility: ±0.001 mole fraction (authors).

References:


---

Components: Original Measurements:

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water: H₂O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

Variables: Prepared By:

One temperature: 298.15 K

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

Experimental Data

Solubility of water in toluene

<table>
<thead>
<tr>
<th>t/K</th>
<th>g(2)/100 g sln (compiler)</th>
<th>x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.15</td>
<td>0.00092</td>
<td>0.0047</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

Source and Purity of Materials:

(1) Aldrich Chemical Co., purity 99.8 mass %; purity >99.8 mass % checked by glc; µ<sup>H</sup> 0.86235; used as received.
(2) Wako Pure Chemical, purity 99.9 mass %, µ<sup>H</sup> 0.99602.

Estimated Error:

Solubility: ±0.001 mole fraction (authors).
### Experimental Data

**Solubility of water in toluene**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>(10^3 x_2) (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>−9</td>
<td>0.1</td>
<td>0.002</td>
</tr>
<tr>
<td>0.1</td>
<td>0.3</td>
<td>0.005</td>
</tr>
<tr>
<td>1.0</td>
<td>0.020</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>0.034</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>0.053</td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>0.070</td>
<td></td>
</tr>
<tr>
<td>4.9</td>
<td>0.097</td>
<td></td>
</tr>
<tr>
<td>15.8</td>
<td>0.312</td>
<td></td>
</tr>
<tr>
<td>20.8</td>
<td>0.413</td>
<td></td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Equipment/Procedure:**
Alexejew’s method was used (Alexejew\(^1\)). No additional details were reported in the paper.

**Source and Purity of Materials:**
1. Kahlbaum, CP; dried over calcium chloride and distilled from sodium; purity not specified.
2. Not specified.

**Estimated Error:**
Solubility: ±0.01% (not specified).

**References:**

---

### Experimental Data

**Solubility of toluene in water**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>mol (1)/L sln</th>
<th>g(1)/100 g sln (compiler)</th>
<th>(s_1) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>6.28 (\times) 10(^{-3})</td>
<td>5.81 (\times) 10(^{-2})</td>
<td>1.135 (\times) 10(^{-4})</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Source and Purity of Materials:**
1. Source not specified; purity >99 mole % checked by high-temperature g.l.c.
2. Source not specified.

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

**References:**
Components: Original Measurements:
(1) Toluene: C₇H₈ [108-88-3]
(2) Water: H₂O; [7732-18-5]

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

Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^5 x₁ (compiler)</th>
<th>g(1/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>7.20</td>
<td>0.0368 ± 0.0002</td>
</tr>
<tr>
<td>22</td>
<td>9.62</td>
<td>0.0492 ± 0.0003</td>
</tr>
</tbody>
</table>

Solubility of water in toluene

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^5 x₂ (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>2.18</td>
<td>0.0426 ± 0.0011</td>
</tr>
<tr>
<td>22</td>
<td>2.68</td>
<td>0.0526 ± 0.0016</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by titration. The solubility of (2) in (1) was determined by Clifford’s (Clifford¹) method. Dried air was passed through the vessel with a saturated solution of (2) in (1) and U-tubes with CaCl₂, and next absorbed (2) was weighed.

Source and Purity of Materials:
(1) Source not specified; boiling point 109.8 °C at 752 mmHg, d²₄₀=0.8636, and d₂₀=0.8743.
(2) Not specified.

Estimated Error:
Solubility: see experimental values above.

References:

Components: Original Measurements:
(1) Toluene: C₇H₈ [108-88-3]
(2) Water: H₂O; [7732-18-5]

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

Experimental Data
Solubility of toluene in water

<table>
<thead>
<tr>
<th>T/K</th>
<th>mol (1)/g (2)</th>
<th>g(1)/100 g sln (compiler)</th>
<th>s₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.15</td>
<td>(6.81 ± 0.08)·10⁻⁴</td>
<td>6.27·10⁻⁴</td>
<td>1.226·10⁻⁴</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

Source and Purity of Materials:
(1) Commercial analytical grade reagent; purity >99% by glc; distilled through a column.
(2) Distilled water passed through an Amberlite CG 120 + CG 400 ion-exchange column.

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

References:
### 2.5. Toluene+Heavy Water

**Components:**

(1) Toluene; C\(_7\)H\(_8\); [108-88-3]

(2) Heavy water (deuterium oxide); D\(_2\)O; [7789-20-0]

**Original Measurements:**


**Variables:**

Prepared By:

A. Maczynski and Z. Maczynska

**Experimental Data**

Solubility of heavy water in toluene

<table>
<thead>
<tr>
<th>t (^\circ)C</th>
<th>10(^2) x (_D) (compiler)</th>
<th>g (2)/100 g sln (compiler)</th>
<th>mol (2)/L sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1.71</td>
<td>0.0372</td>
<td>0.0162</td>
</tr>
<tr>
<td>25</td>
<td>2.31</td>
<td>0.0504</td>
<td>0.0213</td>
</tr>
<tr>
<td>30</td>
<td>2.57</td>
<td>0.0560</td>
<td>0.0240</td>
</tr>
</tbody>
</table>

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

**Auxiliary Information**

**Source and Purity of Materials:**

(1) Source not specified; reagent grade; purified by distillation and dried over molecular sieve.

(2) Distilled in a pyrex system.

**Estimated Error:**

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

---

**Method/Apparatus/Procedure:**

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

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

Components: Cycloheptene; C₇H₁₂; 628-92-2
Water; H₂O; 7732-18-5

Variables:
One temperature: 25 °C

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

Experimental Data
The solubility of cycloheptene in water at 25 °C was reported to be 66 mg (1)/kg (2).
The corresponding mass percent and mole fraction, x₁, calculated by the compilers are 0.0066 (1)/100 g sln and 1.2 × 10⁻⁵.

Auxiliary Information

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

Estimated Error:
Temperature: ± 1.5 °C.
Solubility: 4 mg (1)/kg (2) (standard deviation of mean).

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

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

Estimated Error:
Temperature: ± 1.5 °C.
Solubility: 4 mg (1)/kg (2) (standard deviation of mean).

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in Khazanov.¹

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

Estimated Error:
Not specified.

References:
### 2.7. 1,6-Heptadiene + Water

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H(_2)O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>One temperature: 25 °C</td>
<td>A. Maczynski, Z. Maczynska, and A. Szafranski</td>
</tr>
</tbody>
</table>

**Experimental Data**

The solubility of 1,6-heptadiene in water at 25 °C was reported to be 44 mg (1)/100 g (2). The corresponding mass percent and mole fraction, \(x_1\), calculated by the compilers are 0.0044 g (1)/100 g sln and 8.2 \(\times\) 10\(^{-6}\).

**Auxiliary Information**

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

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

### 2.8. 1-Heptyne + Water

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H(_2)O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>One temperature: 25 °C</td>
<td>A. Maczynski, Z. Maczynska, and A. Szafranski</td>
</tr>
</tbody>
</table>

**Experimental Data**

The solubility of 1-heptyne in water at 25 °C was reported to be 94 mg (1)/100 g (2). The corresponding mass percent and mole fraction, \(x_1\), calculated by the compilers are 0.0094 g (1)/100 g sln and 1.76 \(\times\) 10\(^{-5}\).

**Auxiliary Information**

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Temperature: ±1.5 °C.
Solubility: 3 mg (1)/kg (2) (standard deviation of mean).
2.9. 1-Methylcyclohexene + Water

Components:
(1) 1-Methylcyclohexene; C₇H₁₂; [591-49-1]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C

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

Experimental Data

The solubility of 1-methylcyclohexene in water at 25 °C was reported to be 52 mg (1)/100 g (2).

The corresponding mass percent and mole fraction, x₁, calculated by the compilers are 0.0052 g (1)/100 g sln and 9.7 × 10⁻⁶.

Auxiliary Information

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

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

Estimated Error:
Temperature: ± 1.5 °C
Solubility: 52 mg (1)/kg (2) (standard deviation of mean).

2.10. Cycloheptane + Water

Components:
(1) Cycloheptane; C₇H₁₄; [291-64-5]
(2) Water; H₂O; [7732-18-5]

Evaluators:

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

The experimental solubility data for (1) in (2) have been investigated by Groves¹ at 303 K, and McAuliffe² 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:

\[ \ln x_{1} = \ln x_{\text{min},1} + \frac{\Delta_{\text{sol}} C_{p}}{R} \left( \frac{T}{T_{\text{min}}} - \ln \left( \frac{T_{\text{min}}}{T} \right) - 1 \right) \]

where \( \ln x_{\text{min},1} = -12.45, \Delta_{\text{sol}} C_{p} = 42.6, \) and \( T_{\text{min}} = 298 \) K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data.

Comparison between Reference and experimental data is one of the criteria used to assign data to categories.

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

References:

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

<table>
<thead>
<tr>
<th>T/K</th>
<th>Experimental values ( x_{1} ) (T = tentative)</th>
<th>Reference values ( x_{1} ) ± 30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>298.2</td>
<td>5.50 × 10⁻⁶ (T; Ref. 2)</td>
<td>4.3 × 10⁻⁶</td>
</tr>
<tr>
<td>303.2</td>
<td>4.99 × 10⁻⁶ (T; Ref. 1)</td>
<td>4.3 × 10⁻⁶</td>
</tr>
</tbody>
</table>
Components:
(1) Cycloheptane; C₇H₁₄; [291-64-5]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 30.0 °C

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

---

Experimental Data

Solubility of cycloheptane in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>mg (1)/L sln</th>
<th>g(1)/100 g sln (compilers)</th>
<th>x₁ (compilers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.0</td>
<td>27 ± 1.4</td>
<td>0.00272</td>
<td>4.99 × 10⁻⁶</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

Source and Purity of Materials:
(1) Aldrich, Chemical Co.; purity 98%; used as received.
(2) Distilled.

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

References:

---

Components:
(1) Cycloheptane; C₇H₁₄; [291-64-5]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

---

Experimental Data

The solubility of cycloheptane in water at 25 °C was reported to be 30 mg (1)/kg sln [0.0030 g(1)/100 g sln]. The corresponding mole fraction, x₁, calculated by the compiler, is 5.5 × 10⁻⁶. The same value is also reported in McAuliffe.¹

Auxiliary Information

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

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

Estimated Error:
Temperature: ±1.5 °C
Solubility: 1.0 mg (1)/kg sln (standard deviation of mean).

References:
### 2.11. Ethylcyclopentane+Water

**Components:**
(1) Ethylcyclopentane; C\(_7\)H\(_{14}\); [1640-89-7]
(2) Water; H\(_2\)O; [7732-18-5]

**Original Measurements:**

**Variables:**
- Prepared By: A. Maczynski and M. C. Haulait-Pirson
- Temperature: 10 °C–30 °C

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>(10^{-2} x_1) (compiler)</th>
<th>(g(1)/100) g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.87</td>
<td>0.0071</td>
</tr>
<tr>
<td>20</td>
<td>6.49</td>
<td>0.0119</td>
</tr>
<tr>
<td>30</td>
<td>10.14</td>
<td>0.0186</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- 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.
  - Component (2) was prepared by dehydration of water and its purity was not specified.
- Estimated Error:
  Not specified.

---

### 2.11. Ethylcyclopentane+Water

**Components:**
(1) Ethylcyclopentane; C\(_7\)H\(_{14}\); [1640-89-7]
(2) Water; H\(_2\)O; [7732-18-5]

**Original Measurements:**

**Variables:**
- Prepared By: M. C. Haulait-Pirson
- Temperature: 70.5 °C–203 °C

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>(10^{-4} x_1)</th>
<th>(g(1)/100) g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>70.5</td>
<td>0.40</td>
<td>0.0219</td>
</tr>
<tr>
<td>113</td>
<td>0.96</td>
<td>0.0525</td>
</tr>
<tr>
<td>168.5</td>
<td>4.10</td>
<td>0.224</td>
</tr>
<tr>
<td>203</td>
<td>13.89</td>
<td>0.759</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- Source and Purity of Materials:
  - Presumably the measurements were made in sealed glass tubes, as reported in Guseva and Parnov. 3
  - No more details were reported in the paper.
- Estimated Error:
  Not specified.
- References:
### 2.12. 1-Heptene + Water

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

The experimental solubility data for (1) in (2) have been investigated by Natarajan and Venkatachalam\(^3\) at 293 K–303 K and Tewari\ et al.\(^4\) at 298 K.

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

\[
\ln x_1 = \ln x_{1,\text{exp}} + \left( \frac{\Delta_h C_p}{R} \right) \left( \frac{T}{T_{\text{ref}}} - 1 \right),
\]

where \(\ln x_{1,\text{exp}} = -12.94\), \(\Delta_h C_p / R = 51.3\), and \(T_{\text{ref}} = 306\) K.

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

The experimental and reference data of Natarajan and Venkatachalam\(^3\) and Tewari\ et al.\(^4\) are in good agreement (within 30% relative standard deviation) with the reference data and are Doubtful.

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

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

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

\[
\ln x_2 = d_1 + d_2 \left( T_{\text{ref}} - 1 \right) + d_3 \left( 1 - T_{\text{ref}} \right) + d_4 \left( 1 - T_{\text{ref}} \right),
\]

where \(d_1 = -1.090\), \(d_2 = -2.602\), \(d_3 = 1.406\), \(d_4 = -10.43\), and \(T_{\text{ref}} = 275.22\) K.

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

The experimental and reference solubility data for (2) in (1) are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Black\ et al.\(^1\) are in poor agreement with the reference data and are Doubtful.

**References:**


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

<table>
<thead>
<tr>
<th>(T/K)</th>
<th>Experimental values (x_1) (D = doubtful)</th>
<th>Reference values (x_1 \pm 30%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.2</td>
<td>5.70 (\times) 10(-6) (D; Ref. 3)</td>
<td>2.5 (\times) 10(-6)</td>
</tr>
<tr>
<td>298.2</td>
<td>5.10 (\times) 10(-6) (D; Ref. 3)</td>
<td>2.4 (\times) 10(-6)</td>
</tr>
<tr>
<td>303.2</td>
<td>3.34 (\times) 10(-6) (D; Ref. 4)</td>
<td>2.4 (\times) 10(-6)</td>
</tr>
<tr>
<td>308.2</td>
<td>4.40 (\times) 10(-6) (D; Ref. 3)</td>
<td>2.4 (\times) 10(-6)</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>(T/K)</th>
<th>Experimental values (x_2) (T = tentative, D = doubtful)</th>
<th>Reference values (x_2 \pm 30%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>283.2</td>
<td>3.76 (\times) 10(-3) (D; Ref. 1), 1.01 (\times) 10(-3) (T; Ref. 2)</td>
<td>9.1 (\times) 10(-4)</td>
</tr>
<tr>
<td>293.2</td>
<td>1.36 (\times) 10(-3) (T; Ref. 2)</td>
<td>1.3 (\times) 10(-3)</td>
</tr>
<tr>
<td>293.3</td>
<td>6.11 (\times) 10(-3) (D; Ref. 1)</td>
<td>1.3 (\times) 10(-3)</td>
</tr>
<tr>
<td>293.7</td>
<td>5.68 (\times) 10(-3) (D; Ref. 1)</td>
<td>1.3 (\times) 10(-3)</td>
</tr>
<tr>
<td>294.4</td>
<td>6.28 (\times) 10(-3) (D; Ref. 1)</td>
<td>1.3 (\times) 10(-3)</td>
</tr>
<tr>
<td>303.2</td>
<td>2.04 (\times) 10(-3) (T; Ref. 2)</td>
<td>1.8 (\times) 10(-3)</td>
</tr>
</tbody>
</table>
### Experimental Data

Solubility of water in 1-heptene

<table>
<thead>
<tr>
<th>t°C</th>
<th>$10^3 \times x_2$ (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>3.76</td>
<td>0.0692</td>
</tr>
<tr>
<td>20.1</td>
<td>6.11</td>
<td>0.1126</td>
</tr>
<tr>
<td>20.5</td>
<td>5.68</td>
<td>0.1047</td>
</tr>
<tr>
<td>21.2</td>
<td>6.28</td>
<td>0.1158</td>
</tr>
</tbody>
</table>

At total saturation pressure of 1 atm.

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

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

**References:**


---

### Experimental Data

Solubility of water in 1-heptene

<table>
<thead>
<tr>
<th>t°C</th>
<th>$10^3 \times x_2$ (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.01</td>
<td>0.0186</td>
</tr>
<tr>
<td>20</td>
<td>1.36</td>
<td>0.0249</td>
</tr>
<tr>
<td>30</td>
<td>2.04</td>
<td>0.0375</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Not specified.
Components:
1. 1-Heptene; C7H14; [592-76-7]
2. Water; H2O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25.0 °C

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

Experimental Data
Solubility of 1-heptene in water

<table>
<thead>
<tr>
<th>T/°C</th>
<th>mol (1)/L sln</th>
<th>g (1)/100 g sln (compiler)</th>
<th>x1 (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>1.85 x 10^-4</td>
<td>1.82 x 10^-3</td>
<td>3.34 x 10^-6</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
A generator column method was used, described in DeVoe et al. and May et al. 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:

Components:
1. 1-Heptene; C7H14; [592-76-7]
2. Water; H2O; [7732-18-5]

Original Measurements:

Variables:
Temperature: 20 °C–30 °C

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

Experimental Data
Solubility of 1-heptene in 0.001 mol/L HNO3 solution

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^5 x_1 (compiler)</th>
<th>10^3 g (1)/100 g sln^b (compiler)</th>
<th>10^6 mol(1)/L sln^a</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>5.7</td>
<td>3.1</td>
<td>3.16 ± 0.13</td>
</tr>
<tr>
<td>25</td>
<td>5.1</td>
<td>2.8</td>
<td>2.81 ± 0.12</td>
</tr>
<tr>
<td>30</td>
<td>4.4</td>
<td>2.4</td>
<td>2.45 ± 0.15</td>
</tr>
</tbody>
</table>

^aUncertainties stated to be "standard deviations from means."

^bAssuming a solution density of 1.00 g mL^-1 at all temperatures.

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

Auxiliary Information

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

Source and Purity of Materials:
(1) Matheson, Coleman and Bell, 99%. (2) Not specified.

Estimated Error:
Temperature: ± 0.05 °C.
Solubility: see table above.
2.13. 2-Heptene + Water

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

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

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

\[
\ln x_1 = \ln x_{1,\text{ref}} + \frac{\Delta U}{R} \left( \frac{T_{\text{ref}}}{T} - \ln \frac{T_{\text{ref}}}{T} - 1 \right),
\]

where \( \ln x_{1,\text{ref}} = -12.54, \Delta U/R = 49.3, \) and \( T_{\text{ref}} = 300 \) K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data.

Comparison between reference and experimental data is one of the criteria used to assign data to categories.

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

References:
\(^1\)C. McAuliffe, J. Phys. Chem. 70, 1267 (1966).
\(^3\)F. P. Schwarz, Anal. Chem. 52, 10 (1980).

| Table 10. Experimental values for solubility of 2-heptene (1) in water (2) |
|---|---|---|
| \( T/K \) | Experimental values \( x_1 \) \((T=\text{tentative}, D=\text{doubtful})\) | Reference values \( x_1 \pm 30\% \) |
| 296.7 | 2.75 \times 10^{-6} (T; Ref. 3) | 3.7 \times 10^{-6} |
| 298.2 | 2.70 \times 10^{-6} (T; Ref. 1), 4.89 \times 10^{-6} (D; Ref. 2) | 3.6 \times 10^{-6} |

---

Experimental Data

The solubility of 2-heptane in water at 25 °C was reported to be 15 mg (1)/100 g sln and 2.7 \times 10^{-6}.

Auxiliary Information

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

Estimated Error:
Temperature: ±1.5 °C
Solubility: 1.4 mg (1)/100 g sln (standard deviation of mean).
Components:  
1. 2-Heptene; C7H14; [592-77-8]  
2. Water; H2O; [7732-18-5]

Variables:  
One temperature: 23.5 °C

Prepared By:  
M. C. Haulait-Piron

Experimental Data  
The solubility of 2-heptene in water at 23.5 °C was reported to be 0.00150 ± 0.00003 g (1)/100 g sln. The corresponding mole fraction, x_1, calculated by the compiler is 2.75 • 10^{-6}.

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

Source and Purity of Materials:  
1. 99% purity used without further purification.  
2. Distilled.

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

Components:  
1. 2-Heptene; C7H14; [592-77-8]  
2. Water; H2O; [7732-18-5]

Variables:  
One temperature: 25 °C

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

Experimental Data  
The solubility of 2-heptene in water was reported to be 2.716 • 10^{-4} mol • L at 25 °C.a Assuming a solution density of 1.00 g • mL the corresponding mass percent and mole fraction, x_1, solubilities, calculated by the compilers are, respectively, 0.00266 g (1)/100 g sln and 4.89 • 10^{-6}.

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

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

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

Estimated Error:  
Temperature: ± 0.05 °C.  
Solubility: not specified.
2.14. Methylcyclohexane+Water

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

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

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Reference</th>
<th>T/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Groves1</td>
<td>D; Ref. 3</td>
<td>298</td>
</tr>
<tr>
<td>Guseva and Parnov3</td>
<td>D; Ref. 4</td>
<td>341–488</td>
</tr>
<tr>
<td>Hellinger and Sandler4</td>
<td>D; Ref. 6</td>
<td>298–423</td>
</tr>
</tbody>
</table>

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:

\[ \ln x_1 = \ln x_{\text{exp}} + \left( \Delta \mu^G / R \right) \left( T / T_{\text{ref}} - 1 \right) \]

where \( x_{\text{exp}} = -12.85 \), \( \Delta \mu^G = 4.7 \), and \( T_{\text{ref}} = 298 \) K.

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

All the experimental and reference data are listed in Table 11 and shown in Fig. 5. The data of Groves,2 Price,5 and Rudakov and Latysh2 at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. The data of Hellinger and Sandler,4 and McAuliffe2 at 298 K, and Price5 at 313 K–410 K are in good agreement with the reference data and are Tentative. The data of Guseva and Parnov3 at 341 K–488 K and Price5 at 425 K are in poor agreement with the reference data and are Doubtful.

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

The experimental solubility data for (2) in (1) have been investigated by Englin et al.1 at 273 K–303 K, and Hellinger and Sandler5 at 298 K.

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

\[ \ln x_2 = d_1 + d_2 \left( T / T - 1 \right) + d_3 \left( 1 - T / T_{\text{ref}} \right)^2 + d_4 \left( 1 - T / T_{\text{ref}} \right) \]

where \( d_1 = -0.203 \), \( d_2 = -6.277 \), \( d_3 = -1.935 \), \( d_4 = -1.695 \), and \( T_{\text{ref}} = 298 K \).

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

The experimental and reference solubility data for (2) in (1) are listed in Table 12. All the data are in poor agreement with the reference data and are Doubtful.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga6 are independent data.

References:

8T. Krzyzanowska and J. Szeliga, Nafta (Katowice) 12, 413 (1978).
Components:
(1) Methylcyclohexane; C7H14; [108-87-2]
(2) Water; H2O; [7732-18-5]

Variables:
Temperature: 10 °C– 30 °C

Experimental Data
Solubility of water in methylcyclohexane

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^4 x_2 (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.33</td>
<td>0.0061</td>
</tr>
<tr>
<td>20</td>
<td>6.32</td>
<td>0.0116</td>
</tr>
<tr>
<td>30</td>
<td>9.75</td>
<td>0.0179</td>
</tr>
</tbody>
</table>

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.

Experimental Data
Solubility of methylcyclohexane in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>mg (1)/L sln</th>
<th>g(1)/100 g sln (compilers)</th>
<th>x_1 (compilers)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>16.7±0.6</td>
<td>0.00167</td>
<td>3.07·10^-6</td>
</tr>
</tbody>
</table>

Auxiliary Information

Source and Purity of Materials:
(1) Aldrich, Chemical Co.; purity 99%; used as received.
(2) Distilled.

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

References:
Components: (1) Methylcyclohexane; C\(_7\)H\(_{14}\); [108-87-2]
(2) Water; H\(_2\)O; [7732-18-5]


Variables:
Temperature: 68 °C – 215 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data
Solubility of methylcyclohexane in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^a (x_1) (compiler)</th>
<th>g(1)/100 g sln</th>
<th>g(1)/100 g sln (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>68</td>
<td>0.20</td>
<td>0.011</td>
<td>0.011</td>
</tr>
<tr>
<td>120.5</td>
<td>0.67</td>
<td>0.0363</td>
<td>0.0363</td>
</tr>
<tr>
<td>157.5</td>
<td>1.71</td>
<td>0.0933</td>
<td>0.0933</td>
</tr>
<tr>
<td>215</td>
<td>13.90</td>
<td>0.759</td>
<td>0.759</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Presumably the measurements were made in sealed glass tubes, as reported in Guseva and Parnov. No more details were reported in the paper.

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

Estimated Error:
Not specified.

References:

Components: (1) Methylcyclohexane; C\(_7\)H\(_{14}\); [108-87-2]
(2) Water; H\(_2\)O; [7732-18-5]


Variables:
One temperature: 25.0 °C

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

Experimental Data
Solubility of methylcyclohexane in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^5 g(1)/100 g sln (compilers)</th>
<th>10^6 (x_1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>1.27</td>
<td>2.33</td>
</tr>
<tr>
<td></td>
<td>1.43</td>
<td>2.62</td>
</tr>
</tbody>
</table>

Solubility of water in methylcyclohexane

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^5 g(2)/100 g sln (compilers)</th>
<th>10^3 (x_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>3.53</td>
<td>1.92</td>
</tr>
<tr>
<td></td>
<td>1.51</td>
<td>0.82</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

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

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

References:
Components:
(1) Methylcyclohexane; C7H14; [108-87-2]
(2) Water; H2O; [7732-18-5]

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data
The solubility of methylcyclohexane in water at 25 °C was reported to be 14 mg/l/kg sln
The corresponding mole fraction, x1, calculated by the compiler, is 2.6 \times 10^{-6}. The same value is also reported in the two publications by McAuliffe.1,2

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

Estimated Error:
Temperature: ±1.5 °C
Solubility: range of values given above.

References:

Experimental Data
Solubility of methylcyclohexane in water at system pressure

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^6 x_1 (compiler)</th>
<th>g (1)/100 g sln (compiler)</th>
<th>mg (1)/kg (2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>2.9</td>
<td>0.00160</td>
<td>16.0±0.2</td>
</tr>
<tr>
<td>40.1</td>
<td>3.3</td>
<td>0.00180</td>
<td>18.0±0.6</td>
</tr>
<tr>
<td>55.7</td>
<td>3.5</td>
<td>0.00189</td>
<td>18.9±0.5</td>
</tr>
<tr>
<td>99.1</td>
<td>6.2</td>
<td>0.00358</td>
<td>35.8±1.0</td>
</tr>
<tr>
<td>120.0</td>
<td>14.6</td>
<td>0.00795</td>
<td>79.5±2.2</td>
</tr>
<tr>
<td>137.3</td>
<td>25.5</td>
<td>0.01390</td>
<td>139.0±8.0</td>
</tr>
<tr>
<td>149.5</td>
<td>44.8</td>
<td>0.02440</td>
<td>244.0±10.0</td>
</tr>
</tbody>
</table>

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

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

Source and Purity of Materials:
(1) Phillips Petroleum Company; 99+ % purity; used as received.
(2) Distilled.
Components:
1. Methylcyclohexane; C₇H₁₄; [108-87-2]
2. Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data
The authors reported the partition coefficient of methylcyclohexane between the gas and aqueous phase.

Variables: Prepared By:
One temperature: 25 °C M. C. Haulait-Pirson

Experimental Data
The authors reported the partition coefficient of methylcyclohexane between the gas and aqueous phase.

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

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

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

References:

2.15. 2,2-Dimethylpentane + Water

Components:
1. 2,2-Dimethylpentane; C₉H₁₈; [590-35-2]
2. Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

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

Source and Purity of Materials:
(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C
Solubility: ±0.11 mg(1)/kg(2).
2.16. 2,3-Dimethylpentane + Water

Components:
(1) 2,3-Dimethylpentane; C\textsubscript{16}H\textsubscript{34}; [565-59-3]
(2) Water; H\textsubscript{2}O; [7732-18-5]

Original Measurements:

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Piron

Experimental Data
The solubility of 2,3-dimethylpentane in water at 25 °C and at system pressure was reported to be 5.25 mg (1/kg) (2).
The corresponding mass percent and mole fraction, \( x_1 \), calculated by the compiler are 5.25 \( \times 10^{-4} \) g(1)/100 g sln and 9.43 \( \times 10^{-7} \).

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 gc using a Hewlett-Packard model 5701 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

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

Estimated Error:
Temperature: ± 1 °C.
Solubility: ± 0.02 mg(1/kg)(2).

2.17. 2,4-Dimethylpentane + Water

Components:
(1) 2,4-Dimethylpentane; C\textsubscript{16}H\textsubscript{34}; [108-08-7]
(2) Water; H\textsubscript{2}O; [7732-18-5]

Evaluators:

Critical Evaluation of the Solubility of 2,4-Dimethylpentane (1) in Water (2)
The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Author(s)</th>
<th>T/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>McAudiff\textsuperscript{2}</td>
<td>298</td>
<td>Polak and Lu\textsuperscript{3}</td>
<td>273 and 298</td>
</tr>
<tr>
<td>McAudiff\textsuperscript{2}</td>
<td>298</td>
<td>Price\textsuperscript{4}</td>
<td>298</td>
</tr>
</tbody>
</table>

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:

\[ \ln x_1 = \ln x_{\text{exp}} + \left( \Delta_{\text{exp}} C_p / R \right) \left( \frac{T}{T_R} - 1 \right) \]

where \( x_{\text{exp}} = 14.16 \), \( \Delta_{\text{exp}} C_p / R = 51.4 \), and \( T_R = 306 \text{ K} \).

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

All the experimental and reference data are listed in Table 13. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

Critical Evaluation of the Solubility of Water (2) in 2,4-Dimethylpentane (1)
The experimental solubility data for (2) in (1) have been investigated only by Polak and Lu\textsuperscript{3} at 273 K and 298 K.

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

\[ \ln x_2 = \ln x_{\text{exp}} - d_1(1/T - 1) + d_2(1 - T_R / T) \]

where \( d_1 = -0.974 \), \( d_2 = 6.061 \), \( d_3 = -0.081 \), \( d_4 = -4.808 \), and \( T_R = 7509.3 \).

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

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

Rejected and Inaccessible Data
In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga\textsuperscript{3} are independent data.

References:
\textsuperscript{1} C. McAuliffe, Nature (London) 200, 1092 (1963).
\textsuperscript{2} C. McAuliffe, J. Phys. Chem. 70, 1267 (1966).
\textsuperscript{5} T. Krzyzanowska and J. Szeliga, Nafta (Katowice) 12, 413 (1978).

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

<table>
<thead>
<tr>
<th>T/K</th>
<th>( x_1 ) (\textsuperscript{R} recommended, \textsuperscript{T} tentative)</th>
<th>( x_1 \geq 30% )</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.2</td>
<td>1.17 ( \times 10^{-6} ) (T; Ref. 3)</td>
<td>1.1 ( \times 10^{-6} )</td>
</tr>
<tr>
<td>298.2</td>
<td>6.50 ( \times 10^{-7} ) (T; Ref. 1), 7.30 ( \times 10^{-7} ) (T; Ref. 2), 9.88 ( \times 10^{-7} ) (T; Ref. 3)</td>
<td>8.0 ( \times 10^{-7} ) (T; Ref. 4)</td>
</tr>
</tbody>
</table>
The solubility of 2,4-dimethylpentane in water at 25 °C was reported to be 3.62 mg/kg sln. The corresponding mole fraction, \( x_1 \), calculated by the compiler, is \( 6.5 \times 10^{-7} \).

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

<table>
<thead>
<tr>
<th>( T/K )</th>
<th>Experimental values ( x_2 ) (( T = \text{tentative}, D = \text{doubtful} ))</th>
<th>Reference values ( x_2 \pm 30% )</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.2</td>
<td>( 1.73 \times 10^{-4} ) (T; Ref. 3)</td>
<td>( 2.0 \times 10^{-4} )</td>
</tr>
<tr>
<td>298.2</td>
<td>( 4.51 \times 10^{-4} ) (D; Ref. 3)</td>
<td>( 6.6 \times 10^{-4} )</td>
</tr>
</tbody>
</table>

**Experimental Data**

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

**Auxiliary Information**

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Temperature: ±1.5 °C.
Solubility: 0.10 mg (1) in kg sln (standard deviation from mean).
**Experimental Data**

The solubility of 2,4-dimethylpentane in water at 25 °C was reported to be 4.06 mg (1/100 g sln). The corresponding mole fraction, $x_1$, calculated by the compiler, is $7.3 \times 10^{-7}$. The same value is also reported in McAuliffe.1

### Auxiliary Information

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

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

**Estimated Error:**
Temperature: ± 1.5 °C.
Solubility: 0.29 mg (1/100 g sln) ± 1.7% mean.

**References:**
Components:  
(1) 2,4-Dimethylpentane; C₇H₁₆; [108-08-7]  
(2) Water; H₂O; [7732-18-5]

Original Measurements:  

Variables:  
One temperature: 25 °C  
Prepared By:  
M. C. Haulait-Pirson

Experimental Data  
The solubility of 2,4-dimethylpentane in water at 25 °C and at system pressure was reported to be 4.41 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x₁, calculated by the compiler are 4.41 • 10⁻⁴ g(1)/100 g sln and 7.92 • 10⁻⁷.

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

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

Estimated Error:  
Temperature: ± 1 °C.  
Solubility: ± 0.05 mg(1)/kg(2).

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.

Experimental Data  
Solubility of 3,3-dimethylpentane in water at system pressure

<table>
<thead>
<tr>
<th>℃</th>
<th>10^3 x₁ (compiler)</th>
<th>g(1)/100 g sln (compiler)</th>
<th>mg(1)/kg(2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>1.06</td>
<td>0.000592</td>
<td>5.92±0.06</td>
</tr>
<tr>
<td>40.1</td>
<td>1.22</td>
<td>0.000678</td>
<td>6.78±0.20</td>
</tr>
<tr>
<td>55.7</td>
<td>1.47</td>
<td>0.000817</td>
<td>8.17±0.46</td>
</tr>
<tr>
<td>69.7</td>
<td>1.85</td>
<td>0.00103</td>
<td>10.3±0.7</td>
</tr>
<tr>
<td>99.1</td>
<td>2.84</td>
<td>0.00158</td>
<td>15.8±0.7</td>
</tr>
<tr>
<td>118.0</td>
<td>4.91</td>
<td>0.00273</td>
<td>27.3±0.4</td>
</tr>
<tr>
<td>140.4</td>
<td>12.10</td>
<td>0.00673</td>
<td>67.3±1.7</td>
</tr>
<tr>
<td>150.4</td>
<td>15.48</td>
<td>0.00861</td>
<td>86.1±1.8</td>
</tr>
</tbody>
</table>

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

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

Estimated Error:  
Temperature: ± 1 °C.  
Solubility: range of values given above.
2.19. Heptane+Water

Components:

(1) Heptane: C<sub>7</sub>H<sub>16</sub>; [142:82:5]

(2) Water: H<sub>2</sub>O; [7372:18:5]

Evaluators:


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

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

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Author(s)</th>
<th>T/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biritich et al.</td>
<td>298 and 313</td>
<td>Krasnoschevkova and Gubergrits&lt;sup&gt;13&lt;/sup&gt;</td>
<td>298</td>
</tr>
<tr>
<td>Booth and Eversen&lt;sup&gt;4&lt;/sup&gt;</td>
<td>298</td>
<td>McAuliffe&lt;sup&gt;14&lt;/sup&gt;</td>
<td>298</td>
</tr>
<tr>
<td>Budatsheva et al.</td>
<td>293 and 313</td>
<td>McCants et al.&lt;sup&gt;16&lt;/sup&gt;</td>
<td>311</td>
</tr>
<tr>
<td>Durand&lt;sup&gt;6&lt;/sup&gt;</td>
<td>289</td>
<td>Nelson and De Ligny&lt;sup&gt;16&lt;/sup&gt;</td>
<td>277–318</td>
</tr>
<tr>
<td>Fuhler&lt;sup&gt;2&lt;/sup&gt;</td>
<td>280</td>
<td>Poland and Lu&lt;sup&gt;17&lt;/sup&gt;</td>
<td>273 and 298</td>
</tr>
<tr>
<td>Guevra and Parnev&lt;sup&gt;10&lt;/sup&gt;</td>
<td>345–460</td>
<td>Price&lt;sup&gt;13&lt;/sup&gt;</td>
<td>298–424</td>
</tr>
<tr>
<td>Jonsson et al.&lt;sup&gt;11&lt;/sup&gt;</td>
<td>288–308</td>
<td>Rudakov and Lutsyk&lt;sup&gt;19&lt;/sup&gt;</td>
<td>298</td>
</tr>
<tr>
<td>Korotman and Aref'eva&lt;sup&gt;12&lt;/sup&gt;</td>
<td>293</td>
<td>Tewari et al.&lt;sup&gt;21&lt;/sup&gt;</td>
<td>298</td>
</tr>
</tbody>
</table>

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:

\[
\ln \frac{1}{n} = \ln k_{s_{\text{sol}}} + \left( \Delta_{\text{sol}} / R \right) \left( T - T_{\text{ref}} \right) - \frac{1}{T} - 1.
\]

where \( k_{s_{\text{sol}}} \) is the solubility coefficient for hydrocarbons in water and \( T_{\text{ref}} = 298 \) K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of Reference data.

Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 15. All the experimental and reference data are listed in Table 16 and shown in Fig. 6. The Recommended and Tentative data are shown in Fig. 7.

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

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

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>T/K</th>
<th>Author(s)</th>
<th>T/K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biritich et al.</td>
<td>298 and 313</td>
<td>McCants et al.&lt;sup&gt;16&lt;/sup&gt;</td>
<td>311</td>
</tr>
<tr>
<td>Black et al.</td>
<td>283–298</td>
<td>Poland and Lu&lt;sup&gt;17&lt;/sup&gt;</td>
<td>273 and 298</td>
</tr>
<tr>
<td>Budatsheva et al.</td>
<td>293 and 313</td>
<td>Schatzberg&lt;sup&gt;18&lt;/sup&gt;</td>
<td>298</td>
</tr>
<tr>
<td>Englia et al.&lt;sup&gt;13&lt;/sup&gt;</td>
<td>273–323</td>
<td>Zel'vinskii et al.&lt;sup&gt;12&lt;/sup&gt;</td>
<td>296</td>
</tr>
<tr>
<td>Ghanem et al.&lt;sup&gt;9&lt;/sup&gt;</td>
<td>296</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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:

\[
\ln \frac{1}{n} = \ln k_{s_{\text{sol}}} + \left( \Delta_{\text{sol}} / R \right) \left( T - T_{\text{ref}} \right) - \frac{1}{T} - 1.
\]

where \( k_{s_{\text{sol}}} \) is the solubility coefficient for hydrocarbons in water and \( T_{\text{ref}} = 298 \) K.

Equation (1) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of heptane in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 17.

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

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

The experimental high pressure solubility of (1) in (2) have been investigated by Connolly<sup>7</sup> at constant temperatures 568 K–628 K and 17 220 kPa–70 910 kPa. There data were measured by only one author hence have not been critically evaluated.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga<sup>20</sup> are independent data. The data reported by Broili<sup>22</sup> et al.,<sup>23</sup> Gill et al.,<sup>24</sup> Milligan,<sup>25</sup> and Roof<sup>26</sup> lack sufficient information to justify evaluation.

References:

22. T. Krzyzanowska and J. Szeliga, Naftha (Kanowiec) 12, 413 (1978).

Table 15. The data categories for solubility of heptane (1) in water (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Recommended [data in good agreement (± 30%) with each other and with the reference data]</th>
<th>Tentative [data in good agreement (± 30%) with the reference data]</th>
<th>Doubtful [data in poor agreement (± 30%) with the reference data]</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.2</td>
<td>277.5</td>
<td>286.7</td>
<td>Polak and Lu&lt;sup&gt;17&lt;/sup&gt;</td>
</tr>
<tr>
<td>288.2</td>
<td>288.7</td>
<td>289.2</td>
<td>Nelson and De Ligny&lt;sup&gt;16&lt;/sup&gt;</td>
</tr>
<tr>
<td>293.2</td>
<td>293.8</td>
<td>294.3</td>
<td>Jonsson et al.&lt;sup&gt;11&lt;/sup&gt;</td>
</tr>
<tr>
<td>298.2</td>
<td>298.8</td>
<td>299.3</td>
<td>McCants et al.&lt;sup&gt;15&lt;/sup&gt;</td>
</tr>
<tr>
<td>311.0</td>
<td>311.2</td>
<td>313.3</td>
<td>Nelson and De Ligny&lt;sup&gt;16&lt;/sup&gt;</td>
</tr>
<tr>
<td>318.2</td>
<td>328.9</td>
<td>344.7</td>
<td>Price&lt;sup&gt;18&lt;/sup&gt;</td>
</tr>
<tr>
<td>372.3</td>
<td>381.2</td>
<td>391.2</td>
<td>Guseva and Parnov&lt;sup&gt;10&lt;/sup&gt;</td>
</tr>
<tr>
<td>409.8</td>
<td>423.6</td>
<td>454.2</td>
<td>Guseva and Parnov&lt;sup&gt;10&lt;/sup&gt;</td>
</tr>
<tr>
<td>460.2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

IUPAC-NIST SOLUBILITY DATA SERIES
Table 16. Experimental values for solubility of heptane (1) in water (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Experimental values $x_1$</th>
<th>Reference values $x_1 \pm 30%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.2</td>
<td>$7.88 \times 10^{-7}$ (T; Ref. 17)</td>
<td>$7.5 \times 10^{-7}$</td>
</tr>
<tr>
<td>277.5</td>
<td>$3.51 \times 10^{-7}$ (D; Ref. 16)</td>
<td>$6.8 \times 10^{-7}$</td>
</tr>
<tr>
<td>286.7</td>
<td>$3.63 \times 10^{-7}$ (D; Ref. 16)</td>
<td>$5.9 \times 10^{-7}$</td>
</tr>
<tr>
<td>288.2</td>
<td>$4.80 \times 10^{-7}$ (T; Ref. 11)</td>
<td>$5.8 \times 10^{-7}$</td>
</tr>
<tr>
<td>288.7</td>
<td>$9.00 \times 10^{-6}$ (D; Ref. 8)</td>
<td>$5.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>289.2</td>
<td>$1.80 \times 10^{-6}$ (D; Ref. 6)</td>
<td>$5.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>293.2</td>
<td>$3.00 \times 10^{-6}$ (D; Ref. 4), $4.62 \times 10^{-7}$ (T; Ref. 11), $1.10 \times 10^{-7}$ (D; Ref. 12)</td>
<td>$5.3 \times 10^{-7}$</td>
</tr>
<tr>
<td>298.2</td>
<td>$4.90 \times 10^{-5}$ (D; Ref. 9), $4.51 \times 10^{-7}$ (T; Ref. 11), $5.00 \times 10^{-7}$ (R; Ref. 13), $5.30 \times 10^{-7}$ (R; Ref. 14), $3.78 \times 10^{-7}$ (T; Ref. 16), $6.05 \times 10^{-7}$ (T; Ref. 17), $4.00 \times 10^{-7}$ (T; Ref. 18), $5.20 \times 10^{-7}$ (R; Ref. 19), $6.45 \times 10^{-7}$ (T; Ref. 21), $5.2 \times 10^{-7}$ (T; Ref. 11), $4.07 \times 10^{-7}$ (T; Ref. 16)</td>
<td>$5.3 \times 10^{-7}$</td>
</tr>
<tr>
<td>303.2</td>
<td>$4.47 \times 10^{-2}$ (T; Ref. 11), $4.07 \times 10^{-7}$ (T; Ref. 16)</td>
<td>$5.2 \times 10^{-7}$</td>
</tr>
<tr>
<td>311.0</td>
<td>$2.00 \times 10^{-4}$ (D; Ref. 15)</td>
<td>$5.3 \times 10^{-7}$</td>
</tr>
<tr>
<td>313.2</td>
<td>$1.00 \times 10^{-5}$ (D; Ref. 4)</td>
<td>$5.3 \times 10^{-7}$</td>
</tr>
<tr>
<td>313.3</td>
<td>$5.00 \times 10^{-7}$ (T; Ref. 18)</td>
<td>$5.3 \times 10^{-7}$</td>
</tr>
<tr>
<td>318.2</td>
<td>$4.32 \times 10^{-7}$ (T; Ref. 16)</td>
<td>$5.4 \times 10^{-7}$</td>
</tr>
<tr>
<td>328.9</td>
<td>$5.60 \times 10^{-7}$ (T; Ref. 18)</td>
<td>$6.0 \times 10^{-7}$</td>
</tr>
<tr>
<td>344.7</td>
<td>$1.80 \times 10^{-5}$ (D; Ref. 10)</td>
<td>$7.5 \times 10^{-7}$</td>
</tr>
<tr>
<td>372.3</td>
<td>$1.01 \times 10^{-6}$ (T; Ref. 18)</td>
<td>$1.4 \times 10^{-6}$</td>
</tr>
<tr>
<td>381.2</td>
<td>$2.90 \times 10^{-7}$ (D; Ref. 10)</td>
<td>$1.7 \times 10^{-6}$</td>
</tr>
<tr>
<td>391.2</td>
<td>$2.05 \times 10^{-6}$ (T; Ref. 18)</td>
<td>$2.3 \times 10^{-6}$</td>
</tr>
<tr>
<td>409.8</td>
<td>$4.91 \times 10^{-6}$ (T; Ref. 18)</td>
<td>$4.1 \times 10^{-6}$</td>
</tr>
<tr>
<td>423.6</td>
<td>$7.86 \times 10^{-6}$ (T; Ref. 18)</td>
<td>$6.6 \times 10^{-6}$</td>
</tr>
<tr>
<td>454.2</td>
<td>$1.14 \times 10^{-5}$ (D; Ref. 10)</td>
<td>$2.0 \times 10^{-5}$</td>
</tr>
<tr>
<td>460.2</td>
<td>$1.21 \times 10^{-4}$ (D; Ref. 10)</td>
<td>$2.6 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>T/K</th>
<th>Recommended (data in good agreement (±30%) with each other and with the reference data)</th>
<th>Tentative (data in good agreement (±30%) with the reference data)</th>
<th>Doubtful (data in poor agreement (&gt;30%) with the reference data)</th>
</tr>
</thead>
</table>
| 273.2 | Englin et al.
Polak and Lu
Budantseva et al.
Englin et al. |                      |                                           |
| 283.2 | Englin et al.
Black et al.
Englin et al. |                      |                                           |
| 293.2 | Budantseva et al.
Black et al.
Englin et al. |                      |                                           |
| 295.7 |                      | Ghanem et al.
Zel’venskii et al.
Black et al. |                                           |
| 296.2 |                      |                                           |                                           |
| 298.2 |                      |                                           |                                           |
| 303.2 |                      |                                           |                                           |
| 311.0 |                      |                                           |                                           |
| 313.2 |                      |                                           |                                           |
| 323.2 |                      |                                           |                                           |
Table 18. Experimental values for solubility of water (2) in heptane (1)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Experimental values x₂ (R=recommended, T=tentative, D=doubtful)</th>
<th>Reference values x₂±30%</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.2</td>
<td>1.50·10⁻⁴ (T; Ref. 7), 1.45·10⁻⁴ (T; Ref. 17)</td>
<td>1.9·10⁻⁴</td>
</tr>
<tr>
<td>283.2</td>
<td>4.28·10⁻⁴ (D; Ref. 2), 3.00·10⁻⁴ (T; Ref. 7)</td>
<td>3.0·10⁻⁴</td>
</tr>
<tr>
<td>293.2</td>
<td>7.56·10⁻⁴ (D; Ref. 2), 7.00·10⁻⁴ (D; Ref. 2), 5.00·10⁻⁴ (T; Ref. 4), 5.34·10⁻⁴ (T; Ref. 7)</td>
<td>4.8·10⁻⁴</td>
</tr>
<tr>
<td>295.7</td>
<td>3.19·10⁻⁴ (D; Ref. 9)</td>
<td>5.4·10⁻⁴</td>
</tr>
<tr>
<td>296.2</td>
<td>7.73·10⁻⁴ (D; Ref. 22)</td>
<td>5.5·10⁻⁴</td>
</tr>
<tr>
<td>298.2</td>
<td>6.70·10⁻⁴ (T; Ref. 1), 8.39·10⁻⁴ (D; Ref. 2), 4.56·10⁻⁴ (T; Ref. 17), 5.06·10⁻⁴ (T; Ref. 20)</td>
<td>6.0·10⁻⁴</td>
</tr>
<tr>
<td>303.2</td>
<td>9.57·10⁻⁴ (T; Ref. 7)</td>
<td>7.5·10⁻⁴</td>
</tr>
<tr>
<td>311.0</td>
<td>6.60·10⁻³ (D; Ref. 15)</td>
<td>1.0·10⁻³</td>
</tr>
<tr>
<td>313.2</td>
<td>8.70·10⁻⁴ (T; Ref. 1), 7.00·10⁻⁴ (D; Ref. 4), 1.71·10⁻³ (D; Ref. 7)</td>
<td>1.1·10⁻³</td>
</tr>
<tr>
<td>323.2</td>
<td>2.66·10⁻³ (D; Ref. 7)</td>
<td>1.7·10⁻³</td>
</tr>
</tbody>
</table>

Variables:
Temperature: 25 °C–40 °C

Experimental Data
Solubility of heptane in water

<table>
<thead>
<tr>
<th>T/°C</th>
<th>x₁ (compiler)</th>
<th>g(1)/100 g sln (compiler)</th>
<th>mg (1/kg (2))</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.5</td>
<td>6.6·10⁻¹</td>
<td>0.00037</td>
<td>3.7</td>
</tr>
</tbody>
</table>

Solubility of water in heptane

<table>
<thead>
<tr>
<th>T/°C</th>
<th>x₂ (compiler)</th>
<th>g(2)/100 g sln (compiler)</th>
<th>mg (2/kg (1))</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>6.7·10⁻⁴</td>
<td>0.0121</td>
<td>121</td>
</tr>
<tr>
<td>40</td>
<td>8.6·10⁻⁴</td>
<td>0.0156</td>
<td>156</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was shaken in the absence of air at a
specified temperature and then thermostatted for 48 h. The
equilibrated phases were sampled and analyzed by gas
chromatography using a flame ionization detector. A 3 m steel
column of 15% nitrile silicone on Porolith, 110 °C and a 3 m steel
column of 1.5 g CaCl₂ and 10% SE 30 on chromaton N,
120 °C were used for (1) and (2), respectively.

Source and Purity of Materials:
(1) Source not specified; distilled or crystallized; purity tested by
gas chromatography.
(2) Not specified.

Estimated Error:
Solubility: ± 9% (type of error not specified).
Components: Original Measurements:


Variables: Prepared By:
Temperature: 10 °C–25 °C M. C. Haulait-Piron

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

<table>
<thead>
<tr>
<th>(t^\circ\text{C})</th>
<th>(10^4 x_2) (\text{g}(2)/\text{g sln})</th>
<th>(g(2)/100\text{g sln})</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>4.28</td>
<td>0.0077</td>
</tr>
<tr>
<td>20</td>
<td>7.56</td>
<td>0.0136</td>
</tr>
<tr>
<td>25</td>
<td>8.39</td>
<td>0.0151</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The method described in Joris and Taylor\textsuperscript{1} in which tritium oxide acts as a tracer, was used. Air saturated with radioactive water vapor was bubbled through the water until saturation was attained. Dissolved water was separated from the sample by absorption on calcium oxide. The tritium was transferred to the counter through equilibration with ethanol vapor.

Source and Purity of Materials:
(1) Ohio State University under an American Petroleum Institute project; purity not specified; used as received.
(2) Distilled.

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

References:

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

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

Auxiliary Information

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

Source and Purity of Materials:
(1) Highest grade commercial sample available; no other details given.
(2) Distilled.

Estimated Error:
Not specified.
Experimental Data

Solubility of heptane in water

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$10^5 x_1$ (compiler)</th>
<th>$10^5 g$(1)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.3</td>
<td>2</td>
</tr>
<tr>
<td>40</td>
<td>1</td>
<td>6</td>
</tr>
</tbody>
</table>

Solubility of water in heptane

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$10^5 x_2$ (compiler)</th>
<th>$10^5 g$(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>5</td>
<td>9</td>
</tr>
<tr>
<td>40</td>
<td>7</td>
<td>13</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:

Source and Purity of Materials:

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

Estimated Error:

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

Components:
(1) Heptane; C$_7$H$_{16}$; [142-82-5]
(2) Water; H$_2$O; [7732-18-5]

Original Measurements:

Prepared By:
A. Maczynski
The solubility of heptane in water at 16 °C was reported to be 0.015 mL/L.

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

### Experimental Data

**Solubility of water in heptane**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>$10^4 \cdot x_2$ (compiler)</th>
<th>g(2)g100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.50</td>
<td>0.0027</td>
</tr>
<tr>
<td>10</td>
<td>3.00</td>
<td>0.0054</td>
</tr>
<tr>
<td>20</td>
<td>5.34</td>
<td>0.0096</td>
</tr>
<tr>
<td>30</td>
<td>9.57</td>
<td>0.0172</td>
</tr>
<tr>
<td>40</td>
<td>17.1</td>
<td>0.0308</td>
</tr>
<tr>
<td>50</td>
<td>26.6</td>
<td>0.0480</td>
</tr>
</tbody>
</table>

### Auxiliary Information

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

**Source and Purity of Materials:**

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

**Estimated Error:**
Solubility: ±0.005 mL/L.

**References:**

Components:

| (1) Heptane: C7H16; [142-82-5] | (1) Heptane: C7H16; [142-82-5] |

Original Measurements:


Variables:

| One temperature: 15.5 °C | One temperature: 22.5 °C |

Prepared By:

M. C. Haulait-Pirson

M. C. Haulait-Pirson

Experimental Data

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

The corresponding mole fraction, x₁, calculated by the compiler is 0.9 \( \times 10^{-5} \).

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

The corresponding mass percent and mole fraction, x₂, calculated by the compiler are 5.73 \( \times 10^{-3} \) g (2)/100 g sln and 3.19 \( \times 10^{-4} \).

Auxiliary Information

Method/Apparatus/Procedure:

In a stoppered measuring cylinder pipetted volumes of weighed amounts of (1) were added with shaking to 50, 100, or 1000 mL of (2) until a completely clear solution was obtained at the experimental temperature.

Source and Purity of Materials:

(1) Source not specified; commercial grade; used as received.

(2) Not specified.

Estimated Error:

Not specified.

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Source not specified; purified by shaking with a mixture of H2SO4 and P2O5, kept over KOH, then distilled and the distillate refluxed over NaOH; residual water content <5 \( \times 10^{-6} \) mol/L.

(2) Not specified.

Estimated Error:

Temperature: ±1 °C

Solubility: ±10% (type of error not specified).
Components: Original Measurements:

<table>
<thead>
<tr>
<th>Components</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heptane: C₇H₁₆</td>
<td>142-82-5</td>
</tr>
<tr>
<td>Water: H₂O</td>
<td>7732-18-5</td>
</tr>
</tbody>
</table>


Variables:

<table>
<thead>
<tr>
<th>Prepared By</th>
<th>Temperature: 71.5 °C–187 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>A. Maczynski</td>
<td></td>
</tr>
</tbody>
</table>

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁵ x₁ (g/l/100 g sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>71.5</td>
<td>1.8 0.010</td>
</tr>
<tr>
<td>108</td>
<td>2.9 0.016</td>
</tr>
<tr>
<td>181</td>
<td>11.4 0.0635</td>
</tr>
<tr>
<td>187</td>
<td>12.07 0.0671</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in Khazanova.¹

Source and Purity of Materials:

(1) Not specified.
(2) Distilled.

Estimated Error:

Not specified.

References:


---

Components: Original Measurements:

<table>
<thead>
<tr>
<th>Components</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heptane: C₇H₁₆</td>
<td>142-82-5</td>
</tr>
<tr>
<td>Water: H₂O</td>
<td>7732-18-5</td>
</tr>
</tbody>
</table>


Variables:

<table>
<thead>
<tr>
<th>Prepared By</th>
<th>Temperature: 15 °C–35 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>G. T. Hefter</td>
<td></td>
</tr>
</tbody>
</table>

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁷ x₁ (g/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>4.80 2.67</td>
</tr>
<tr>
<td>20</td>
<td>4.62 2.57</td>
</tr>
<tr>
<td>25</td>
<td>4.51 2.51</td>
</tr>
<tr>
<td>30</td>
<td>4.47 2.49</td>
</tr>
<tr>
<td>35</td>
<td>4.53 2.52</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Fluka, >99.7%, used as received.
(2) Not specified.

Estimated Error:

Not specified.

References:

### Experimental Data

**Variables:**

One temperature: 20 °C

**Prepared By:**

A. Maczynski

#### Components:

1. Heptane; C\textsubscript{7}H\textsubscript{16}; [142-82-5]
2. Water; H\textsubscript{2}O; [7732-18-5]

**Original Measurements:**


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

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

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Not specified.

---

### Experimental Data

**Variables:**

One temperature: 25 °C

**Prepared By:**

A. Maczynski

#### Components:

1. Heptane; C\textsubscript{7}H\textsubscript{16}; [142-82-5]
2. Water; H\textsubscript{2}O; [7732-18-5]

**Original Measurements:**


The solubility of heptane in water at 25 °C was reported to be \(s_1 = 5.0 \cdot 10^{-7}\).

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

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Not specified.
<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Heptane; C\textsubscript{7}H\textsubscript{16}; [142-82-5]</td>
<td>C. McAuliffe, J. Phys. Chem. 70, 1267 (1966).</td>
</tr>
</tbody>
</table>

**Variables:**

- One temperature: 25 °C
- One temperature: 100 °F (311 K)

**Prepared By:**

M. C. Haulait-Pirson

G. T. Hefter

---

**Experimental Data**

**The solubility of heptane in water at 25 °C**

The solubility of heptane in water at 25 °C was reported to be 2.93 mg (1)/kg sln [0.000293 g/(1)/100 g sln].

The corresponding mole fraction, $x_1$, calculated by the compiler, is $5.3 \times 10^{-7}$. The same value is also reported in the two papers by McAuliffe. \(^1\)\(^2\)

**Auxiliary Information**

**Method/Apparatus/Procedure:**

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

**Source and Purity of Materials:**

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

**Estimated Error:**

Temperature: ±1.5 °C
Solubility: ±0.20 mg (1)/kg sln (standard deviation of mean).

**References:**


**The solubility of heptane in water at 100 °F (311 K)**

The solubility of heptane in water at 100 °F (311 K) was reported to be $<0.1 g/(1)/100 g sln$.

The corresponding mole fraction, $x_1$, calculated by the compiler, is $2 \times 10^{-4}$.

The solubility of water in heptane at 100 °F (311 K) was reported to be 0.12 g/(2)/100 g sln.

The corresponding mole fraction, $x_2$, calculated by the compiler, is $6.6 \times 10^{-3}$.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The method was essentially that of Washburn et al.\(^3\) and involved titration of the second component to the cloud point, in a constant temperature bath.

**Source and Purity of Materials:**

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

**Estimated Error:**

Not specified.

**References:**

Components: (1) Heptane; C_{7}H_{16}; [142-82-5]
(2) Water; H_{2}O; [7732-18-5]


Variables: Temperature: 4.3 °C–45 °C
Prepared By: M. C. Haulait-Pirson

### Experimental Data

<table>
<thead>
<tr>
<th>temperature/°C</th>
<th>Solubility of heptane in water/10^7 x_1</th>
<th>mg (1/kg sln) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.3</td>
<td>3.51±0.26</td>
<td>1.95</td>
</tr>
<tr>
<td>13.5</td>
<td>3.63±0.51</td>
<td>2.02</td>
</tr>
<tr>
<td>25</td>
<td>4.78±0.74</td>
<td>2.66</td>
</tr>
<tr>
<td>35</td>
<td>4.07±0.95</td>
<td>2.27</td>
</tr>
<tr>
<td>45</td>
<td>4.32±1.06</td>
<td>2.41</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

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

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

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

---

Components: (1) Heptane; C_{7}H_{16}; [142-82-5]
(2) Water; H_{2}O; [7732-18-5]


Variables: Temperature: 0 °C–25 °C
Prepared By: M. C. Haulait-Pirson

### Experimental Data

<table>
<thead>
<tr>
<th>temperature/°C</th>
<th>Solubility of heptane in water/10^7 x_1</th>
<th>mg (1/kg sln) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0^a</td>
<td>7.9</td>
<td>4.39^a</td>
</tr>
<tr>
<td>25^b</td>
<td>6.1</td>
<td>3.37^b</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>temperature/°C</th>
<th>Solubility of water in heptane/10^4 x_2</th>
<th>mg (2/kg sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0^a</td>
<td>1.45</td>
<td>26^d</td>
</tr>
<tr>
<td>25^b</td>
<td>4.56</td>
<td>82^e</td>
</tr>
</tbody>
</table>

^a See Estimated Error.

**Auxiliary Information**

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

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

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

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

The compiler has assumed that when (1) and (2) are not very soluble in each other, \( C_s \) may be taken as the water solubility and \( C_g \) as the vapor pressure of (1). The value of \( P \) where \( P = 45.81 \text{ mm of Hg} \) is taken from Ref. 1.

\[
C_s = 2.9 \times 10^{-5} \text{ moles/L}.
\]

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent is 0.00029 \( g/100 \text{ g sln} \) and the corresponding mole fraction, \( x_1 \), is 5.2 \( \times 10^{-3} \).

Auxiliary Information

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

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

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

References:
Components:
(1) Heptane; C\textsubscript{7}H\textsubscript{16}; [142-82-5]
(2) Water; H\textsubscript{2}O; [7732-18-5]

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data
The solubility of water in heptane at 25 °C was reported to be 91 mg (2)/kg sln corresponding to a mole fraction, x\textsubscript{2}, of 5.06 \times 10^{-4} and to a mass percent of 0.0091 g(1)/100 g sln.

Auxiliary Information

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

Source and Purity of Materials:
(1) Eastman Organic Chemicals; doubly distilled; passed repeatedly through a column of silica gel until no absorption occurred in the 220–340 nm spectral range.
(2) Distilled and deionized.

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

Reference:
### 2.20. Heptane + Heavy Water

#### Components:
- (1) Heptane; C\textsubscript{7}H\textsubscript{16}; [142-82-5]
- (2) Deuterium oxide (heavy water); D\textsubscript{2}O; [7789-20-0]

#### Original Measurements:

#### Variables:
- Temperature: 68 °C–193 °C

#### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10\textsuperscript{3} x_1</th>
<th>g (1/100 g sln) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>68</td>
<td>1.51</td>
<td>0.0076</td>
</tr>
<tr>
<td>109</td>
<td>2.8</td>
<td>0.0140</td>
</tr>
<tr>
<td>158</td>
<td>6.24</td>
<td>0.0312</td>
</tr>
<tr>
<td>193</td>
<td>14.9</td>
<td>0.0745</td>
</tr>
</tbody>
</table>

#### Auxiliary Information

- **Method/Apparatus/Procedure**: The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in Khazanova.\(^1\)
- **Source and Purity of Materials**:
  - (1) Not specified.
  - (2) Distilled.
- **Estimated Error**: Not specified.

#### References:
2.21. 2-Methylhexane+Water

Components:
(1) 2-Methylhexane; C7H16; [591-76-4]
(2) Water; H2O; [7732-18-5]

Original Measurements:

Variables:
Temperature: 10 °C–30 °C

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

Experimental Data
Solubility of water in 2-methylhexane

<table>
<thead>
<tr>
<th>°C</th>
<th>10^3 x1 (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.12</td>
<td>0.0056</td>
</tr>
<tr>
<td>20</td>
<td>5.73</td>
<td>0.0103</td>
</tr>
<tr>
<td>30</td>
<td>10.12</td>
<td>0.0182</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

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

Estimated Error:
Not specified.

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data
The solubility of 2-methylhexane in water at 25 °C and at system pressure was reported to be 2.54 mg (1)kg (2).

The corresponding mass percent and mole fraction, x1, calculated by the compiler are 2.54·10^-4 (1)/100 g sln and 4.57·10^-7.

Auxiliary Information

Source and Purity of Materials:
(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C
Solubility: ±0.02 mg(1)kg(2).


2.22. 3-Methylhexane+Water

The experimental solubility data for (1) can be found in Table 19 and Table 20, and the reference solubility data for (2) can be found in Table 19. The solubility data were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

\[ \ln x_1 = \ln x_{01} + \Delta \ln C_p / R [\ln (T_{min} / T) - \ln (T_{ref} / T)] \]

where \( \ln x_{01} = -14.21, \Delta \ln C_p / R = 0.789, \) and \( T_{ref} = 306 K. \)

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.

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

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

\[ \ln x_2 = \ln x_{02} + \Delta \ln C_p / R [\ln (T_{min} / T) - \ln (T_{ref} / T)] \]

where \( \ln x_{02} = -3.835, \Delta \ln C_p / R = 6.140, \) and \( T_{ref} = 520.6 K. \)

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

The experimental and reference solubility data for (2) in Table 20 are in good agreement with the reference data and are Tentative. The remaining data at 298 K are in poor agreement with the reference data and are Doubtful.

Rejected and Inaccessible Data

In the opinion of the evaluators, uncertainty exists as to whether the solubility measurements reported by Krzyzanowski and Szeliga are independent data.

References:

Table 19. Experimental values for solubility of 3-methylhexane (1) in water (2)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Experimental values ( x_1 ) (T=tentative, D=doubtful)</th>
<th>Reference values ( x_1 \pm 30% )</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.2</td>
<td>9.41 \times 10^{-7} (T; Ref. 1)</td>
<td>1.1 \times 10^{-6}</td>
</tr>
<tr>
<td>298.2</td>
<td>8.89 \times 10^{-7} (T; Ref. 1) 4.70 \times 10^{-7} (D; Ref. 2)</td>
<td>7.7 \times 10^{-7}</td>
</tr>
</tbody>
</table>

Table 20. Experimental values for solubility of water (2) in 3-methylhexane (1)

<table>
<thead>
<tr>
<th>T/K</th>
<th>Experimental values ( x_2 ) (T; Ref. 1)</th>
<th>Reference values ( x_2 \pm 30% )</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.2</td>
<td>1.39 \times 10^{-4}</td>
<td>1.9 \times 10^{-4}</td>
</tr>
<tr>
<td>298.2</td>
<td>4.12 \times 10^{-4} (D; Ref. 1)</td>
<td>6.1 \times 10^{-4}</td>
</tr>
</tbody>
</table>
### Components:
1. 3-Methylhexane; C7H16; 589-34-4
2. Water; H2O; 7732-18-5

### Original Measurements:

### Variables:
- Temperature: 0 °C–25 °C

### Experimental Data

#### Solubility of 3-methylhexane in water

<table>
<thead>
<tr>
<th>t/°C</th>
<th>(10^2 x_1) (compiler)</th>
<th>mg (1/kg sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>9.41</td>
<td>5.24</td>
</tr>
<tr>
<td>25°</td>
<td>8.89</td>
<td>4.95</td>
</tr>
</tbody>
</table>

#### Solubility of water in 3-methylhexane

<table>
<thead>
<tr>
<th>t/°C</th>
<th>(10^2 x_2) (compiler)</th>
<th>mg (2/kg sln)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>1.39</td>
<td>25</td>
</tr>
<tr>
<td>25°</td>
<td>4.12</td>
<td>74</td>
</tr>
</tbody>
</table>

*See Estimated Error*

### Auxiliary Information

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

- **Source and Purity of Materials:**
  (1) Phillips Petroleum Co.; Chemical Samples Company or Aldrich Chemical Company; 99% + %; shaken three times with distilled water.
  (2) Distilled.

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

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

- **Source and Purity of Materials:**
  (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99% + %.
  (2) Distilled.

- **Estimated Error:**
  Temperature: ± 1 °C.
  Solubility: ± 0.08 mg (1/kg) (2).
### 2.23. 2,2,3-Trimethylbutane + Water

<table>
<thead>
<tr>
<th>Component</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

#### Variables:
- **Temperature**: 0 °C–50 °C
- **Prepared By**: A. Maczynski and M. C. Haulait-Pirson

#### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10³ x₁ (compiler)</th>
<th>g(2)/100 g sln</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.50</td>
<td>0.0027</td>
</tr>
<tr>
<td>10</td>
<td>3.17</td>
<td>0.0057</td>
</tr>
<tr>
<td>20</td>
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<td>30</td>
<td>10.23</td>
<td>0.0184</td>
</tr>
<tr>
<td>40</td>
<td>17.51</td>
<td>0.0315</td>
</tr>
<tr>
<td>50</td>
<td>28.15</td>
<td>0.0507</td>
</tr>
</tbody>
</table>

#### Auxiliary Information

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

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

**Estimated Error:**
- Not specified.
### 3. System Index

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

<table>
<thead>
<tr>
<th>Compound</th>
<th>System</th>
<th>Water Reference Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3,5-Cycloheptatriene</td>
<td></td>
<td>E1402, 1403–1404</td>
</tr>
<tr>
<td>1,6-Heptadiyne</td>
<td></td>
<td>1404</td>
</tr>
<tr>
<td>2,5-Norbornadiene</td>
<td></td>
<td>1405</td>
</tr>
<tr>
<td>Toluene</td>
<td></td>
<td>E1405–E1412, 1412–1445</td>
</tr>
<tr>
<td>Toluene + heavy water</td>
<td></td>
<td>1445–1446</td>
</tr>
<tr>
<td>Cycloheptene</td>
<td></td>
<td>1446</td>
</tr>
<tr>
<td>1,6-Heptadiene + water</td>
<td></td>
<td>1447</td>
</tr>
<tr>
<td>1-Heptyne + water</td>
<td></td>
<td>1447</td>
</tr>
<tr>
<td>1-Methylcyclohexene + water</td>
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</tr>
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<td>Cycloheptane + water</td>
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<td>E1448, 1449</td>
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<td>2-Heptene + water</td>
<td></td>
<td>E1454, 1454–1455</td>
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<tr>
<td>Methylcyclohexane + water</td>
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<td>E1456, 1457–1460</td>
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<td>2,2-Dimethylpentane + water</td>
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<td>1460</td>
</tr>
<tr>
<td>2,3-Dimethylpentane + water</td>
<td></td>
<td>1461</td>
</tr>
<tr>
<td>2,4-Dimethylpentane + water</td>
<td></td>
<td>E1461–E1462, 1462–1464</td>
</tr>
<tr>
<td>3,3-Dimethylpentane + water</td>
<td></td>
<td>1464</td>
</tr>
<tr>
<td>Heptane + water</td>
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<td>E1465–E1467, 1467–1478</td>
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<tr>
<td>Heptane + heavy water</td>
<td></td>
<td>1478</td>
</tr>
<tr>
<td>2-Methylhexane + water</td>
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<td>1479</td>
</tr>
<tr>
<td>3-Methylhexane + water</td>
<td></td>
<td>E1480, 1481</td>
</tr>
<tr>
<td>2,2,3-Trimethylbutane + water</td>
<td></td>
<td>1482</td>
</tr>
</tbody>
</table>

### 4. Registry Number Index

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

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<th>Registry Number</th>
<th>Compound</th>
<th>Registry Number</th>
<th>Registry Number</th>
<th>Registry Number</th>
<th>Registry Number</th>
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<td>C_{7}H_{8} 1,3,5-Cycloheptatriene</td>
<td>2396-63-6</td>
<td>C_{7}H_{8} 1,6-Heptadiyne</td>
<td>121-46-0</td>
<td>C_{7}H_{8} 2,5-Norbornadiene</td>
</tr>
<tr>
<td>108-88-3</td>
<td>C_{7}H_{8} Toluene (Methylbenzene)</td>
<td>628-92-2</td>
<td>C_{7}H_{12} Cycloheptene</td>
<td>3070-53-9</td>
<td>C_{7}H_{12} 1,6-Heptadiene</td>
</tr>
<tr>
<td>628-89-2</td>
<td>C_{7}H_{12} Cycloheptene</td>
<td>628-71-7</td>
<td>C_{7}H_{12} 1-Heptyne</td>
<td>591-49-1</td>
<td>C_{7}H_{12} 1-Methylcyclohexene</td>
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<tr>
<td>291-64-5</td>
<td>C_{7}H_{14} Cycloheptane</td>
<td>1640-89-7</td>
<td>C_{7}H_{14} Ethylcyclopentane</td>
<td>592-76-7</td>
<td>C_{7}H_{14} 1-Heptene</td>
</tr>
<tr>
<td>592-77-8</td>
<td>C_{7}H_{14} 2-Heptene</td>
<td>108-87-2</td>
<td>C_{7}H_{14} Methylcyclohexane</td>
<td>590-35-2</td>
<td>C_{7}H_{16} 2,2-Dimethylpentane</td>
</tr>
<tr>
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<td>C_{7}H_{16} 2,3-Dimethylpentane</td>
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<td>C_{7}H_{16} 2,4-Dimethylpentane</td>
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<td>142-82-5</td>
<td>C_{7}H_{16} Heptane</td>
<td>591-76-4</td>
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