

COMPONENTS: (1) 2,2-Dimethylbutane; C <sub>6</sub> H <sub>14</sub> ; [75-83-2] (2) Water; H <sub>2</sub> O; [7732-18-5]	EVALUATOR: M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984
--	---

## CRITICAL EVALUATION:

Quantitative solubility data for the system 2,2-dimethylbutane (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the  
2,2-Dimethylbutane (1) - Water (2) System

Reference	T/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
Polak and Lu (ref 2)	273,298	mutual	GLC, Karl Fischer
Price (ref 3)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 4)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

## 1. THE SOLUBILITY OF 2,2-DIMETHYLBUTANE (1) IN WATER (2)

The solubility data for 2,2-dimethylbutane in water are listed in Table 2. The datum of Krzyzanowska and Szeliga (ref 4) has been excluded from this evaluation as it does not appear to be independent of that of Price (ref 3). The agreement between the other reported values at 298K (ref 1, 2, 3) is only fair ( $\pm 10\%$  relative) and the average "best" value can only be regarded as tentative at this stage. It should also be noted that the increase in solubility as the temperature goes from 298K to 273K reported by Polak and Lu (ref 2) is larger than typically observed in hydrocarbon-water systems (e.g. benzene in water).

TABLE 2: Tentative Values of the Solubility  
of 2,2-Dimethylbutane (1) in Water (2)

T/K	Solubility values		
	Reported values 10 <sup>3</sup> g(1)/100g sln	"Best" values ( $\pm \sigma_n$ ) <sup>a</sup> 10 <sup>3</sup> g(1)/100g sln	10 <sup>6</sup> x <sub>1</sub>
273	3.94 (ref 2)	3.9	8.2
298	1.84 (ref 1), 2.38 (ref 2), 2.11 (ref 3)	2.1 $\pm$ 0.2	4.4

<sup>a</sup>Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance  
(continued next page)

<p>COMPONENTS:</p> <p>(1) 2,2-Dimethylbutane; C<sub>6</sub>H<sub>14</sub>; [75-83-2]</p> <p>(2) Water; H<sub>2</sub>O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984</p>
<p>CRITICAL EVALUATION: (continued)</p> <p>2. THE SOLUBILITY OF WATER (2) IN 2,2-DIMETHYLBUTANE (1)</p> <p>The solubility of water in 2,2-dimethylbutane has been reported in only one publication (ref 2), and thus no Critical Evaluation can be made. However, the data of Polak and Lu are generally in good agreement with "Recommended" values in well characterized systems. The interested user is referred to the appropriate data sheet for solubility values.</p> <p>REFERENCES</p> <ol style="list-style-type: none"><li>1. McAuliffe, C. <i>J. Phys. Chem.</i> <u>1966</u>, <i>70</i>, 1267-75.</li><li>2. Polak, J.; Lu, B.C-Y. <i>Can. J. Chem.</i> <u>1973</u>, <i>51</i>, 4018-23.</li><li>3. Price, L.C. <i>Am. Assoc. Petrol. Geol. Bull.</i> <u>1976</u>, <i>60</i>, 213-44.</li><li>4. Krzyzanowska, T.; Szeliga, J. <i>Nafta (Katowice)</i> <u>1978</u>, <i>34</i>, 413-7.</li></ol>	

<b>COMPONENTS:</b>  (1) 2,2-Dimethylbutane; C <sub>6</sub> H <sub>14</sub> ; [75-83-5]  (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  McAuliffe, C.  <i>J. Phys. Chem.</i> <u>1966</u> , <i>70</i> , 1267-75.
<b>VARIABLES:</b>  One temperature: 25°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b>  <p>The solubility of 2,2-dimethylbutane in water at 25°C was reported to be 18.4 mg (1)/kg sln (0.00184 g(1)/100 g sln).</p> <p>The corresponding mole fraction, <math>x_1</math>, calculated by the compiler, is <math>3.85 \times 10^{-6}</math>.</p> <p>The same value is also reported in refs 1 and 2.</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr 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 $\mu$ L 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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Phillips Petroleum Co.; 99+% purity; used as received.  (2) distilled.  <b>ESTIMATED ERROR:</b>  temp. $\pm$ 1.5 K soly. 1.3 mg (1)/kg sln (standard deviation from mean)  <b>REFERENCES:</b>  1. McAuliffe, C. <i>Nature (London)</i> <u>1963</u> , <i>200</i> , 1092.  2. McAuliffe, C. <i>Am. Chem. Soc. Div. Petrol. Chem.</i> <u>1964</u> , <i>9</i> , 275.

<b>COMPONENTS:</b> (1) 2,2-Dimethylbutane; C <sub>6</sub> H <sub>14</sub> ; [75-83-2] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Polak, J.; Lu, B.C-Y. <i>Can. J. Chem.</i> <u>1973</u> , <i>51</i> , 4018-23.																		
<b>VARIABLES:</b> Temperature: 0-25°C	<b>PREPARED BY:</b> M.C. Haulait-Pirson																		
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of 2,2-dimethylbutane in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(1)/kg sln</u></th> <th style="text-align: center;"><u>x<sub>1</sub> (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0<sup>a</sup></td> <td style="text-align: center;">39.4<sup>c</sup></td> <td style="text-align: center;">8.23 x 10<sup>-6</sup></td> </tr> <tr> <td style="text-align: center;">25<sup>b</sup></td> <td style="text-align: center;">23.8<sup>c</sup></td> <td style="text-align: center;">4.97 x 10<sup>-6</sup></td> </tr> </tbody> </table> <p style="text-align: center;">Solubility of water in 2,2-dimethylbutane</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>mg(2)/kg sln</u></th> <th style="text-align: center;"><u>x<sub>2</sub> (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0<sup>a</sup></td> <td style="text-align: center;">32<sup>d</sup></td> <td style="text-align: center;">1.53 x 10<sup>-4</sup></td> </tr> <tr> <td style="text-align: center;">25<sup>b</sup></td> <td style="text-align: center;">84<sup>e</sup></td> <td style="text-align: center;">4.02 x 10<sup>-4</sup></td> </tr> </tbody> </table> <p>a<sup>-e</sup> see "ESTIMATED ERROR"</p>		<u>t/°C</u>	<u>mg(1)/kg sln</u>	<u>x<sub>1</sub> (compiler)</u>	0 <sup>a</sup>	39.4 <sup>c</sup>	8.23 x 10 <sup>-6</sup>	25 <sup>b</sup>	23.8 <sup>c</sup>	4.97 x 10 <sup>-6</sup>	<u>t/°C</u>	<u>mg(2)/kg sln</u>	<u>x<sub>2</sub> (compiler)</u>	0 <sup>a</sup>	32 <sup>d</sup>	1.53 x 10 <sup>-4</sup>	25 <sup>b</sup>	84 <sup>e</sup>	4.02 x 10 <sup>-4</sup>
<u>t/°C</u>	<u>mg(1)/kg sln</u>	<u>x<sub>1</sub> (compiler)</u>																	
0 <sup>a</sup>	39.4 <sup>c</sup>	8.23 x 10 <sup>-6</sup>																	
25 <sup>b</sup>	23.8 <sup>c</sup>	4.97 x 10 <sup>-6</sup>																	
<u>t/°C</u>	<u>mg(2)/kg sln</u>	<u>x<sub>2</sub> (compiler)</u>																	
0 <sup>a</sup>	32 <sup>d</sup>	1.53 x 10 <sup>-4</sup>																	
25 <sup>b</sup>	84 <sup>e</sup>	4.02 x 10 <sup>-4</sup>																	
<b>AUXILIARY INFORMATION</b>																			
<b>METHOD/APPARATUS/PROCEDURE:</b>  The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by 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 hr 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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.  <b>ESTIMATED ERROR:</b> temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 1.7%; d) ± 4.7%; e) ± 3.1% (mean)  <b>REFERENCES:</b>																		

<b>COMPONENTS:</b>  (1) 2,2-Dimethylbutane; C <sub>6</sub> H <sub>14</sub> ; [75-83-2]  (2) Water, H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Price, L.C.  <i>Am. Assoc. Petrol. Geol. Bull.</i> . . <u>1976</u> , 60, 213-44.
<b>VARIABLES:</b>  One temperature: 25°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b>  <p>The solubility of 2,2-dimethylbutane in water at 25°C and at system pressure was reported to be 21.1 mg(1)/kg(2). The corresponding mass percent and mole fraction, <math>x_1</math>, calculated by the compiler are 0.00212 g(1)/100 g sln and <math>4.43 \times 10^{-6}</math>.</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%.  (2) distilled.  <b>ESTIMATED ERROR:</b>  temp. $\pm$ 1 K soly. $\pm$ 0.3 mg(1)/kg(2)  <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) 2,2-Dimethylbutane; C <sub>6</sub> H <sub>14</sub> ; [75-83-2] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Krzyzanowska, T.; Szeliga, J. <i>Nafta (Katowice)</i> <u>1978</u> , 12, 413-7.
<b>VARIABLES:</b> One temperature: 25°C	<b>PREPARED BY:</b> M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b> <p>The solubility of 2,2-dimethylbutane in water at 25°C was reported to be 21.20 mg(1)/kg(2).</p> <p>The corresponding mass percent and mole fraction, <math>x_1</math>, calculated by compiler are 0.00212 g(1)/100 g sln and <math>4.43 \times 10^{-6}</math>.</p> <p>Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainty exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b> Saturated solutions of (1) in (2) were prepared in two ways. First, 200 $\mu$ L of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) not specified. (2) not specified.  <b>ESTIMATED ERROR:</b> soly. 1.2 mg(1)/kg(2) (standard deviation from 7-9 determinations)  <b>REFERENCES:</b>