

COMPONENTS: (1) 1,2,4-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6] (2) Water; H <sub>2</sub> O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985.
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CRITICAL EVALUATION:

Quantitative solubility data for 1,2,4-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of  
1,2,4-Trimethylbenzene (1) in Water (2)

Reference	T/K	Method
McAuliffe (ref 1)	298	GLC
Sutton and Calder (ref 2)	298	GLC
Price (ref 3)	298	GLC
Krzyzanowska and Szeliga (ref 4)	298	GLC
Sanemasa <i>et al.</i> (ref 5)	288-318	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data have been reported for the solubility of water in 1,2,4-trimethylbenzene.

All the available data are collected in Table 2 with the exception of that of Krzyzanowska and Szeliga (ref 4) which does not appear to be independent of that of Price (ref 3) and thus has been excluded from consideration. At 298K the only temperature where comparison is possible, the data are in excellent agreement so that the mean can be Recommended, although interestingly the value of Price (ref 3) is somewhat lower than those reported by other workers as for many of the higher hydrocarbons investigated by this author. At other temperatures only the data of Sanemasa *et al.* (ref 5) are available and must thus be regarded as Tentative.

TABLE 2: Recommended (R) and Tentative Values of the Solubility  
of 1,2,4-Trimethylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 <sup>3</sup> g(1)/100g sln	"Best" values (±σ <sub>n</sub> ) <sup>a</sup> 10 <sup>3</sup> g(1)/100g sln	10 <sup>6</sup> x <sub>1</sub>
288	5.23 (ref 5)	5.2	7.8
298	5.7 (ref 1), 5.90 (ref 2), 5.19 (ref 3), 5.65 (ref 5)	5.6 ± 0.3 (R)	8.4 (R)
308	6.21 (ref 5)	6.2	9.3
318	6.93 (ref 5)	6.9	10

<sup>a</sup> Obtained by averaging where appropriate; σ<sub>n</sub> has no statistical significance. (continued next page)

<p>COMPONENTS:</p> <p>(1) 1,2,4-Trimethylbenzene; C<sub>9</sub>H<sub>12</sub>; [95-63-6]</p> <p>(2) Water; H<sub>2</sub>O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.</p> <p>August 1985</p>
<p>CRITICAL EVALUATION: (continued)</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. Sutton, C.; Calder, J.A. <i>J. Chem. Eng. Data</i> <u>1975</u>, <i>20</i>, 320-2.</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><li>5. Sanemasa, I.; Deguchi, T.; Nagai, H. <i>Bull. Chem. Soc. Jpn.</i> <u>1982</u>, <i>55</i>, 1054-62.</li></ol>	

<b>COMPONENTS:</b>  (1) 1,2,4-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6]  (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>  A. Maczynski, Z. Maczynska, and A. Szafranski
<b>EXPERIMENTAL VALUES:</b>  The solubility of 1,2,4-trimethylbenzene in water at 25°C was reported to be 57 g(1)/10 <sup>6</sup> g(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are 0.0057 g(1)/100 g sln and $8.5 \times 10^{-6}$ .	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  In a 250-mL 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. 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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Phillips Petroleum or Columbia Chemical; used as received.  (2) distilled.  <b>ESTIMATED ERROR:</b> temp. $\pm 1.5^\circ\text{C}$ soly. 4 g(1)/10 <sup>6</sup> g(2) (standard deviation of mean)  <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) 1,2,4-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Sutton, C.; Calder, J.A.  <i>J. Chem. Eng. Data</i> 1975, 20, 320-2.
<b>VARIABLES:</b> One temperature: 25°C	<b>PREPARED BY:</b> A. Maczynski and Z. Maczynska
<b>EXPERIMENTAL VALUES:</b>  The solubility of 1,2,4-trimethylbenzene in water at 25°C was reported to be 59.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are 0.00590 g(1)/100 g sln and $8.83 \times 10^{-6}$ .	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  The concentration of (1) in (2) was determined by gas chromatography.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.  (2) distilled.  <b>ESTIMATED ERROR:</b> temp. $\pm$ 0.1°C soly. 0.8 mg(1)/kg(2) (the standard deviation of the mean for six replicates)  <b>REFERENCES:</b>

<b>COMPONENTS:</b>  (1) 1,2,4-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6]  (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>  The solubility of 1,2,4-trimethylbenzene in water at 25°C and at system pressure was reported to be 51.9 mg(1)/kg(2). The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are 0.00519 g(1)/100 g sln and $7.77 \times 10^{-6}$ .	
<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 Aldrich Chemical Company; 99+%.  (2) distilled.  <b>ESTIMATED ERROR:</b>  temp. $\pm 1^\circ\text{C}$ soly. $\pm 1.2 \text{ mg(1)/kg(2)}$  <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) 1,2,4-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6] (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 1,2,4-trimethylbenzene in water at 25°C was reported to be 51.9 mg(1)/kg(2).</p> <p>The corresponding mass percent and mole fraction, <math>x_1</math>, calculated by compiler are 0.00519 g(1)/100 g sln and <math>7.78 \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> <p>The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL 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.</p>	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) not specified. (2) not specified.
<b>ESTIMATED ERROR:</b> soly. 1.6 mg(1)/kg(2) (standard deviation from 7-9 determinations).	
<b>REFERENCES:</b>	

<b>COMPONENTS:</b> (1) 1,2,4-Trimethylbenzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. <i>Bull. Chem. Soc. Jpn.</i> <u>1982</u> , <i>55</i> , 1054-62.																				
<b>VARIABLES:</b> Temperature: 15-45°C	<b>PREPARED BY:</b> G.T. Hefter																				
<b>EXPERIMENTAL VALUES:</b> <p style="text-align: center;">The solubility of 1,2,4-trimethylbenzene in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><math>t / ^\circ\text{C}</math></th> <th style="text-align: center;"><math>10^4 \text{ mol(1)/dm}^3 \text{ sln}</math></th> <th style="text-align: center;"><math>10^3 \text{ g(1)/100 g sln}</math> (compiler)<sup>a</sup></th> <th style="text-align: center;"><math>10^6 x_1</math> (compiler)<sup>a</sup></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">15</td> <td style="text-align: center;">4.35 ± 0.12</td> <td style="text-align: center;">5.23</td> <td style="text-align: center;">7.84</td> </tr> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">4.69 ± 0.07</td> <td style="text-align: center;">5.65</td> <td style="text-align: center;">8.48</td> </tr> <tr> <td style="text-align: center;">35</td> <td style="text-align: center;">5.14 ± 0.20</td> <td style="text-align: center;">6.21</td> <td style="text-align: center;">9.32</td> </tr> <tr> <td style="text-align: center;">45</td> <td style="text-align: center;">5.71 ± 0.07</td> <td style="text-align: center;">6.93</td> <td style="text-align: center;">10.4</td> </tr> </tbody> </table> <p><sup>a</sup> Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).</p>		$t / ^\circ\text{C}$	$10^4 \text{ mol(1)/dm}^3 \text{ sln}$	$10^3 \text{ g(1)/100 g sln}$ (compiler) <sup>a</sup>	$10^6 x_1$ (compiler) <sup>a</sup>	15	4.35 ± 0.12	5.23	7.84	25	4.69 ± 0.07	5.65	8.48	35	5.14 ± 0.20	6.21	9.32	45	5.71 ± 0.07	6.93	10.4
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<b>METHOD/APPARATUS/PROCEDURE:</b> <p>The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm<sup>3</sup> of (2) and 10-20 cm<sup>3</sup> of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm<sup>3</sup> aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.</p>	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 95.0%, used without further purification. (2) Redistilled; no further details given.  <b>ESTIMATED ERROR:</b> soly. see table, type of error not specified. temp. ± 0.01°C.  <b>REFERENCES:</b> 1. Kell, G.S. <i>J. Chem. Eng. Data</i> <u>1975</u> , <i>20</i> , 97. 2. Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. <i>Chem. Lett.</i> <u>1981</u> , 225-8.																				

<b>COMPONENTS:</b> (1) 1,2,4-Trimethylbenzene; $C_9H_{12}$ ; [95-63-6] (2) Artificial seawater (ref 1)	<b>ORIGINAL MEASUREMENTS:</b> Sutton, C.; Calder, J.A. <i>J. Chem. Eng. Data</i> <u>1975</u> , 20, 320-2.
<b>VARIABLES:</b> One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	<b>PREPARED BY:</b> M. Kleinschmidt
<b>EXPERIMENTAL VALUES:</b> <p>The solubility of 1,2,4-trimethylbenzene in artificial seawater is reported to be 39.6 mg(1)/kg sln. The corresponding mass percent and mole fraction, <math>x_1</math> calculated by the compiler are <math>3.96 \times 10^{-3}</math> g(1)/100 g sln and <math>6.09 \times 10^{-6}</math> assuming the artificial seawater composition of ref 1.</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b> <p>A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.</p>	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure.  <b>ESTIMATED ERROR:</b> temp. $\pm$ 0.1°C soly. 0.5 (std. dev.)  <b>REFERENCES:</b> 1. Lyman, J.; Fleming, R.H.; <i>J. Mar. Res.</i> <u>1940</u> , 3, 135.