

COMPONENTS:	EVALUATOR:
(1) 1,2,3-Trimethylbenzene; C ₉ H ₁₂ ; [526-73-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H ₂ O; [7732-18-5]	December 1986

CRITICAL EVALUATION:

Quantitative solubility data for 1,2,3-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1,2,3-trimethylbenzene.

TABLE 1: Quantitative Solubility Studies of 1,2,3-Trimethylbenzene (1) in Water (2)

Reference	T/K	Method
Sutton and Calder (ref 1)	298	GLC
Sanemasa <i>et al.</i> (ref 2)	288-318	spectrophotometry

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The available data are summarized in Table 2. At 298K, the only temperature where comparison is possible, the data of Sutton and Calder (ref 1) and Sanemasa *et al.* (ref 2) are in reasonable agreement (Table 2) and their average may be considered as the Tentative solubility.

At other temperatures, only the data of Sanemasa *et al.* are available so no Critical Evaluation is possible. Nevertheless, it may be noted that for other hydrocarbons in water the data of Sanemasa *et al.* are normally reliable.

TABLE 2: Tentative Values of the Solubility of 1,2,3-Trimethylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ³ g(1)/100g sln	"Best" values (± σ _n) ^a 10 ³ g(1)/100g sln	10 ⁶ x ₁
288	5.99 (ref 2)	6.0	9.0
298	7.52 (ref 1), 6.27 (ref 2)	6.9 ± 0.5	10
308	7.22 (ref 2)	7.2	11
318	8.52 (ref 2)	8.5	13

^a Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

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<p>CRITICAL EVALUATION: (continued)</p> <p>REFERENCES</p> <ol style="list-style-type: none">1. Sutton, C.; Calder, J.A. <i>J. Chem. Eng. Data</i> <u>1975</u>, <i>20</i>, 320-2.2. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. <i>Bull. Chem. Soc. Jpn.</i> <u>1982</u>, <i>55</i>, 1054-62.	

COMPONENTS: (1) 1,2,3-Trimethylbenzene; C ₉ H ₁₂ ; [526-73-8] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Sutton, C.; Calder J.A. <i>J. Chem. Eng. Data</i> <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: The solubility of 1,2,3-trimethylbenzene in water at 25°C was reported to be 75.2 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.00752 g(1)/100 g sln and 1.126×10^{-5} .	
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 purified by distillation through a Vigreux Column; 94.4% purity determined by gas chromatography. (2) Distilled. ESTIMATED ERROR: Temp. ±0.1°C Soly. 0.6 (the standard deviation of the mean for six replicates). REFERENCES:

COMPONENTS: (1) 1,2,3-Trimethylbenzene; C ₉ H ₁₂ ; [526-73-8] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. <i>Bull. Chem. Soc. Jpn.</i> <u>1982</u> , <i>55</i> , 1054-62.																				
VARIABLES: Temperature: 15-45°C	PREPARED BY: G.T. Hefter																				
EXPERIMENTAL VALUES: <p style="text-align: center;">The solubility of 1,2,3-trimethylbenzene in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><i>t</i> / °C</th> <th style="text-align: center;">10⁴ mol(1)/dm³ sln</th> <th style="text-align: center;">10³ g(1)/100 g sln (compiler)^a</th> <th style="text-align: center;">10⁶ <i>x</i>₁ (compiler)^a</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">15</td> <td style="text-align: center;">4.98 ± 0.19</td> <td style="text-align: center;">5.99</td> <td style="text-align: center;">8.97</td> </tr> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">5.20 ± 0.32</td> <td style="text-align: center;">6.27</td> <td style="text-align: center;">9.40</td> </tr> <tr> <td style="text-align: center;">35</td> <td style="text-align: center;">5.97 ± 0.41</td> <td style="text-align: center;">7.22</td> <td style="text-align: center;">10.8</td> </tr> <tr> <td style="text-align: center;">45</td> <td style="text-align: center;">7.02 ± 0.19</td> <td style="text-align: center;">8.52</td> <td style="text-align: center;">12.8</td> </tr> </tbody> </table> <p>^a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).</p>		<i>t</i> / °C	10 ⁴ mol(1)/dm ³ sln	10 ³ g(1)/100 g sln (compiler) ^a	10 ⁶ <i>x</i> ₁ (compiler) ^a	15	4.98 ± 0.19	5.99	8.97	25	5.20 ± 0.32	6.27	9.40	35	5.97 ± 0.41	7.22	10.8	45	7.02 ± 0.19	8.52	12.8
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AUXILIARY INFORMATION																					
METHOD/APPARATUS/PROCEDURE: The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm ³ of (2) and 10-20 cm ³ 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 ³ aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.	SOURCE AND PURITY OF MATERIALS: (1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), no stated purity, used without further purification. (2) Redistilled; no further details given. ESTIMATED ERROR: soly. see table, type of error not specified. temp. ± 0.01°C. REFERENCES: 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.																				

COMPONENTS: (1) 1,2,3-Trimethylbenzene; C_9H_{12} ; [526-73-8] (2) Artificial seawater (ref 1)	ORIGINAL MEASUREMENTS: Sutton, C.; Calder, J.A. <i>J. Chem. Eng. Data</i> <u>1975</u> , 20, 320-2.
VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	PREPARED BY: M. Kleinschmidt
EXPERIMENTAL VALUES: <p>The solubility of 1,2,3-trimethylbenzene in artificial seawater is reported to be 48.6 mg(l)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 4.86×10^{-3} g(l)/100 g sln and 7.47×10^{-6} assuming the artificial seawater composition of ref 1.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure. (2) made from doubly distilled water and salts 99+% pure. ESTIMATED ERROR: temp. \pm 0.1°C soly. 0.5 (std. dev.) REFERENCES: 1. Lyman, J.; Fleming, R.H.; <i>J. Mar. Res.</i> <u>1940</u> , 3, 135.