

<p>COMPONENTS:</p> <p>(1) <i>tert</i>-Butylbenzene; C₁₀H₁₄; [98-06-6]</p> <p>(2) Water; H₂O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland</p> <p>February 1986.</p>
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CRITICAL EVALUATION:

Quantitative solubility data for the *tert*-butylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Solubility Studies of the *tert*-Butylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Englin <i>et al.</i> (ref 2)	283-303	(2) in (1)	analytical
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

The original data in all of the above 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. SOLUBILITY OF *TERT*-BUTYLBENZENE (1) IN WATER (2)

The two reported solubilities of *tert*-butylbenzene in water are in reasonable agreement (Table 2).

TABLE 2: Tentative Value of the Solubility of *tert*-Butylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ³ g(1)/100g sln	"Best" value (± σ _n) ^a 10 ³ g(1)/100g sln	10 ⁶ x ₁
298	3.4 (ref 1), 2.95 (ref 3)	3.2 ± 0.2	4.3

^a Obtained by averaging, σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN *TERT*-BUTYLBENZENE (1)

As only the solubility values of Englin *et al.* (ref 2) are available no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al.* are generally reliable at *T* < 300K but somewhat too high at greater temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

(continued next page)

<p>COMPONENTS:</p> <p>(1) <i>tert</i>-Butylbenzene; C₁₀H₁₄; [98-06-6]</p> <p>(2) Water; H₂O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland</p> <p>February 1986.</p>
<p>CRITICAL EVALUATION: (continued)</p> <p>REFERENCES</p> <ol style="list-style-type: none">1. Andrews, L.J.; Keefer, T.M. <i>J. Am. Chem. Soc.</i> <u>1950</u>, <i>72</i>, 5034-7.2. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u>, <i>10</i>, 42-6.3. Sutton, C.; Calder, J.A. <i>J. Chem. Eng. Data</i> <u>1975</u>, <i>20</i>, 320-2.	

COMPONENTS: (1) tert-Butylbenzene; $C_{10}H_{14}$; [98-06-6] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Andrews, L.J.; Keefer, R.M. <i>J. Am. Chem. Soc.</i> <u>1950</u> , <i>72</i> , 5034-7.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: The solubility of tert-butylbenzene in water at 25°C was reported to be 0.0034 g(1)/100 g sln. The corresponding mole fraction, x_1 calculated by the compilers is 4.6×10^{-6} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: A mixture of (1) and (2) was rotated for twenty hours 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 the Beckman spectrophotometer.	SOURCE AND PURITY OF MATERIALS: (1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 167.8-168.0°C. (2) not specified. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: (1) tert-Butylbenzene; C ₁₀ H ₁₄ ; [98-06-6] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , 10, 42-6.												
VARIABLES: Temperature: 10-30°C	PREPARED BY: A. Maczynski and Z. Maczynska												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of Water in tert-Butylbenzene</p> <table style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;">$t/^{\circ}\text{C}$</th> <th style="text-align: center;">$\text{g}(2)/100 \text{ g sln}$</th> <th style="text-align: center;">$10^3 x_2$ (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">10</td> <td style="text-align: center;">0.0205</td> <td style="text-align: center;">2.03</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0292</td> <td style="text-align: center;">2.88</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.0389</td> <td style="text-align: center;">3.83</td> </tr> </tbody> </table>		$t/^{\circ}\text{C}$	$\text{g}(2)/100 \text{ g sln}$	$10^3 x_2$ (compiler)	10	0.0205	2.03	20	0.0292	2.88	30	0.0389	3.83
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10	0.0205	2.03											
20	0.0292	2.88											
30	0.0389	3.83											
AUXILIARY INFORMATION													
METHOD/APPARATUS/PROCEDURE: Component (1) was introduced into a thermostatted flask and saturated for 5 hr. 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. REFERENCES:												

COMPONENTS: (1) tert-Butylbenzene; C ₁₀ H ₁₄ ; [98-06-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Sutton, C.; Calder, J.A. <i>J. Chem. Eng. Data</i> 1975, 20, 320-2.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: <p>The solubility of tert-butylbenzene in water at 25°C was reported to be 29.5 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00295 g(1)/100 g sln and 3.95×10^{-6}.</p>	
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: temp. $\pm 0.1^\circ\text{C}$ soly. 0.3 (the standard deviation of the mean for six replicates).
	REFERENCES:

COMPONENTS: (1) tert-Butylbenzene; C ₁₀ H ₁₄ ; [98-06-6] (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 and W. Shiu
EXPERIMENTAL VALUES: <p>The solubility of tert-butylbenzene in artificial seawater is reported to be 21.2 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 2.12×10^{-3} g(1)/100 g sln and 2.92×10^{-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. 0.3 (std. dev.) REFERENCES: 1. Lyman, J.; Fleming, R.H.; <i>J. Mar. Res.</i> <u>1940</u> , 3, 135.