

COMPONENTS:

(1) Butylbenzene; C₁₀H₁₄; [104-51-8](2) Water; H₂O; [7732-18-5]

EVALUATOR:

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February 1986.

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Klevens (ref 2)	298	(1) in (2)	spectrophotometric
Jones and Monk (ref 3)	298-308	(2) in (1)	radiotracer
Englin <i>et al.</i> (ref 4)	283-303	(2) in (1)	analytical
Massaldi and King (ref 5)	298	(1) in (2)	GLC
Sutton and Calder (ref 6)	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 BUTYLBENZENE (1) IN WATER (2)

The available data on the solubility of butylbenzene in water, all at 298K, are summarized in Table 2. The agreement is very poor with the reported values differing by almost two orders of magnitude which makes critical evaluation difficult. Fortunately, an independent estimation of the solubility can be made by extrapolation of the solubilities of the lower *n*-alkylbenzenes as a function of side chain length. This extrapolation predicts a value of 1.7×10^{-3} g(1)/100g sln. This value is quite close to the experimental values of Massaldi and King (ref 5) and Sutton and Calder (ref 6), the average of which is therefore suggested as the Tentative solubility of butylbenzene in water. The values of Andrews and Keefer (ref 1) and Klevens (ref 2) are correspondingly rejected.

(continued next page)

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CRITICAL EVALUATION: (continued)

TABLE 2: Solubility of Butylbenzene (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
298	0.126 ^b (ref 1), 4.9 ^b (ref 2) 1.77 (ref 5), 1.18 (ref 6)	1.5 ± 0.3 ^c	2.0

^a Obtained by averaging but see text; σ_n has no statistical significance.^b Rejected data, see text.^c Tentative value, see text.

2. SOLUBILITY OF WATER (2) IN BUTYLBENZENE (1)

Although two publications report solubility data of water in butylbenzene, that of Jones and Monk (ref 3) is reported in v/v fractions and is thus excluded from consideration. The remaining data of Englin *et al.* (ref 4) cannot therefore be evaluated. However it may be noted that the values of Englin *et al.* are usually reliable at $T < 300\text{K}$ but somewhat too high at greater temperatures. The interested user is referred to the relevant data sheet for the experimental values.

REFERENCES

- Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
- Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
- Jones, J.R.; Monk, C.B. *J. Chem. Soc.* 1963, 2633-5.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
- Massaldi, H.A.; King, C.J. *J. Chem. Eng. Data* 1973, *18*, 393-7.
- Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.

COMPONENTS: (1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Andrews, L.J.; Keefer, R.M. <i>J. Am. Chem. Soc.</i> 1950, 72, 5034-7.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: The solubility of butylbenzene in water at 25°C was reported to be 0.000126 g(1)/100 g sln. The corresponding mole fraction, x_1 , calculated by the compilers is 1.69×10^{-7} .	
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. best grade; fractionally distilled; b.p. range 182.0-183.0°C. (2) not specified. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS: (1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Klevens, H.B. <i>J. Phys. Chem.</i> <u>1950</u> , 54, 283-98.
VARIABLES: Temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: <p>The solubility of butylbenzene in water at 25°C was reported to be 0.05 g(1) L⁻¹ sln and 0.00037 mol(1) L⁻¹ sln. Assuming that 1.00 kg sln = 1.00 L sln the mass percentage and mole fraction x_1 calculated by the compilers are 0.005 g(1)/100 g sln and 6.7×10^{-6}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.</p>	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. <hr/> ESTIMATED ERROR: not specified. <hr/> REFERENCES:

COMPONENTS: (1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Jones, J.R.; Monk, C.B. <i>J. Chem. Soc.</i> <u>1963</u> , 2633-35.								
VARIABLES: Temperature: 25-35°C	PREPARED BY: A. Maczynski, Z. Maczynska and A. Szafranski								
EXPERIMENTAL VALUES: <p style="text-align: center;">The solubility of water in butylbenzene</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">10^4 mL (2)/mL (1)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">3.5</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">4.1</td> </tr> <tr> <td style="text-align: center;">35</td> <td style="text-align: center;">4.9</td> </tr> </tbody> </table>		$t/^\circ C$	10^4 mL (2)/mL (1)	25	3.5	30	4.1	35	4.9
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25	3.5								
30	4.1								
35	4.9								
AUXILIARY INFORMATION									
METHOD/APPARATUS/PROCEDURE: In a thermostatted glass-stoppered flask 10-25 mL (1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mc/mL), decanted, a 5-mL aliquot reshaken for 4 hrs. with 5 mL H_2O 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) laboratory grade dried over $CaCl_2$ and fractionally distilled. (2) not specified. ESTIMATED ERROR: soly. \pm 5% to \pm 1% (average deviation) REFERENCES: 1. Vogel <i>Practical Organic Chemistry</i> Longmans, Green and Co., London, <u>1956</u> .								

COMPONENTS: (1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O ; [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 Butylbenzene</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th>$t/^\circ C$</th> <th>$g(2)/100\text{ g sln}$</th> <th>$10^3 x_2$ (compiler)</th> </tr> </thead> <tbody> <tr> <td>10</td> <td>0.0234</td> <td>1.74</td> </tr> <tr> <td>20</td> <td>0.0331</td> <td>2.46</td> </tr> <tr> <td>30</td> <td>0.0448</td> <td>3.33</td> </tr> </tbody> </table>		$t/^\circ C$	$g(2)/100\text{ g sln}$	$10^3 x_2$ (compiler)	10	0.0234	1.74	20	0.0331	2.46	30	0.0448	3.33
$t/^\circ C$	$g(2)/100\text{ g sln}$	$10^3 x_2$ (compiler)											
10	0.0234	1.74											
20	0.0331	2.46											
30	0.0448	3.33											
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) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Massaldi, H.A.; King, C.J. <i>J. Chem. Eng. Data</i> <u>1973</u> , 18, 393-7.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: <p>The solubility of butylbenzene in water at 25°C was reported to be 1.32×10^{-4} mol(1) dm⁻³ sln.</p> <p>The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00177 g(1)/100 g sln and 2.4×10^{-6}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>A technique based on head-space analysis by gas-liquid chromatography was developed to determine solubilities of sparingly soluble organics. Saturated solutions need not be prepared in advance whereby phase separation problems are avoided, nor have liquid samples to be analyzed. This method is versatile enough to allow determinations provided that the pure vapor pressure of the substances is known. The gas chromatograph was a Varian Aerograph Model 1740 with a flame ionization detector.</p>	SOURCE AND PURITY OF MATERIALS: (1) Matheson Coleman and Bell Co., highest purity; used as received. (2) not specified. ESTIMATED ERROR: temp. $\pm 0.05^\circ\text{C}$ REFERENCES:

COMPONENTS: (1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8] (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 butylbenzene in water at 25°C was reported to be 11.8 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00118 g(1)/100 g sln and 1.58×10^{-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. 0.1 mg(1)/kg(2) (the standard deviation of the mean for six replicates) REFERENCES:

COMPONENTS: (1) Butylbenzene; C ₁₀ H ₁₄ ; [104-51-8] (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 and W. Shiu
EXPERIMENTAL VALUES: <p>The solubility of butylbenzene in artificial seawater is reported to be 7.09 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 7.09×10^{-4} g(1)/kg sln and 9.76×10^{-7} 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. 0.07 (std. dev.) REFERENCES: 1. Lyman, J.; Fleming, R.H.; <i>J. Mar. Res.</i> <u>1940</u> , 3, 135.