

COMPONENTS: (1) <i>p</i> -Cymene; C ₁₀ H ₁₄ ; [99-87-5] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.
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CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the *p*-Cymene (1) - Water (2) System

Reference	T/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	volumetric
Englin <i>et al.</i> (ref 2)	283-303	(2) in (1)	analytical
Banerjee <i>et al.</i> (ref 3)	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. SOLUBILITY OF *p*-CYMENE (1) IN WATER (2)

Only two solubility values are available, both at 298K, but they are in poor agreement. The value of 0.04g(1)/100g sln reported by Booth and Everson (ref 1) is more than an order of magnitude greater than the value of 2.34×10^{-3} g(1)/100g sln reported by Banerjee *et al.* (ref 3). On the basis of comparison with similar systems the value of Banerjee *et al.* is more realistic.

2. SOLUBILITY OF WATER (2) IN *p*-CYMENE (1)

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

REFERENCES

1. Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
2. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Khim. Tekhnol. Topl. Masei* 1965, *10*, 42-6.
3. Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.

COMPONENTS: (1) p-Cymene; C ₁₀ H ₁₄ ; [99-87-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Booth, H.S.; Everson, H.E. <i>Ind. Eng. Chem.</i> <u>1948</u> , 40, 1491-3.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES: <p>The solubility of p-cymene in water at 25°C was reported to be 0.04 g(1)/100 mL(2). Assuming a solution density of 1.00, the mass percentage and mole fraction, x_1, calculated by the compilers are 0.04 g(1)/100 g sln and 5×10^{-5}.</p>	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: <p>Stoppered Babcock tubes with neck graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in a constant-temperature water bath and weighed quantities of (1) were added to this solution. The mixture was then shaken for 5 minutes, returned to the bath for a minimum of 10 minutes and then centrifuged for 5 minutes. After this treatment, the volume of residue was determined directly.</p>	SOURCE AND PURITY OF MATERIALS: (1) source not specified; CP or highest commercial grade; used as received. (2) distilled.
ESTIMATED ERROR: soly. \pm 0.1 mL(1)/100 mL(2).	
REFERENCES:	

COMPONENTS: (1) p-Cymene; C ₁₀ H ₁₄ ; [99-87-6] (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 p-Cymene</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>g(2)/100 g sln</u></th> <th style="text-align: center;"><u>10³ x₂ (compiler)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">10</td> <td style="text-align: center;">0.0223</td> <td style="text-align: center;">1.66</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0305</td> <td style="text-align: center;">2.27</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.0415</td> <td style="text-align: center;">3.08</td> </tr> </tbody> </table>		<u>t/°C</u>	<u>g(2)/100 g sln</u>	<u>10³ x₂ (compiler)</u>	10	0.0223	1.66	20	0.0305	2.27	30	0.0415	3.08
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10	0.0223	1.66											
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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) <i>p</i> -Cymene; C ₁₀ H ₁₄ ; [99-87-5] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. <i>Environ. Sci. Technol.</i> <u>1980</u> , <i>14</i> , 1227-9.
VARIABLES: One temperature: 25°C	PREPARED BY: G.T. Hefter
EXPERIMENTAL VALUES: The solubility of <i>p</i> -cymene in water was reported to be 1.74×10^{-4} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction, x_1 , solubilities, calculated by the compiler, are 2.34×10^{-3} g(l)/100 g sln and 3.13×10^{-6} respectively.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: Experiments were performed in sealed stainless steel centrifuge tubes. An excess of <i>p</i> -cymene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at $25 \pm 0.2^\circ\text{C}$ with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to $25 \pm 0.3^\circ\text{C}$, following which aliquots of the solution were removed for analysis by GC after exhaustive extraction with hexane. A HP 5370A (FID) instrument and a 3% OV-1 on Chromosorb W column was used. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.	SOURCE AND PURITY OF MATERIALS: (1) Aldrich; purity not specified. (2) Distilled. ESTIMATED ERROR: Temperature: $\pm 0.2^\circ\text{C}$ Solubility: $\pm 3.1\%$ rel. (representing one std. dev.) REFERENCES: