

COMPONENTS: (1) Triphenylene; C ₁₈ H ₁₂ ; [217-59-4] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.
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CRITICAL EVALUATION:

Quantitative solubility data for triphenylene (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 triphenylene.

TABLE 1. Quantitative Solubility Studies of Triphenylene (1) in Water (2)

Reference	T/K	Method
Davis <i>et al.</i> (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The reported data which are summarized in Table 2 are in excellent agreement. However the solubility values are not sufficiently well characterized, at this stage, to justify Recommending the average value.

TABLE 2. Tentative Solubility Value of Triphenylene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ⁶ g(1)/100 g sln	"Best" value 10 ⁶ g(1)/100 g sln	10 ⁹ x ₁
298	4.28 (ref 2), 4.3 (ref 3)	4.3	3.4
300	3.8 ^a (ref 1)	-	-

^a Datum not sufficiently well characterized to justify inclusion in "best" values.

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
- Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
- Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS: (1) Triphenylene; C ₁₈ H ₁₂ ; [217-59-4] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. <i>J. Am. Chem. Soc.</i> <u>1942</u> , <i>64</i> , 108-10.								
VARIABLES: One temperature: 27°C	PREPARED BY: M.C. Haulait-Pirson								
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of triphenylene in water</p> <table 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>10⁵ g(1) L⁻¹ (2)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">27</td> <td style="text-align: center;">3.8 ± 0.8</td> </tr> <tr> <td></td> <td style="text-align: center;">3.6 ± 0.4</td> </tr> <tr> <td></td> <td style="text-align: center;">4.0 ± 0.4</td> </tr> </tbody> </table> <p>The best value recommended by the authors is 3.8 × 10⁻⁵ g(1) L⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 3.8 × 10⁻⁶ g(1)/100 g sln and 3.0 × 10⁻⁹.</p>		<u>t/°C</u>	<u>10⁵ g(1) L⁻¹ (2)</u>	27	3.8 ± 0.8		3.6 ± 0.4		4.0 ± 0.4
<u>t/°C</u>	<u>10⁵ g(1) L⁻¹ (2)</u>								
27	3.8 ± 0.8								
	3.6 ± 0.4								
	4.0 ± 0.4								
AUXILIARY INFORMATION									
METHOD/APPARATUS/PROCEDURE: The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.	SOURCE AND PURITY OF MATERIALS: (1) prepared at Harvard University; m.p. range 197.5-197.9°C; (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. see above REFERENCES: 1. Davis, W.W.; Parker, Jr., T.V. <i>J. Am. Chem. Soc.</i> <u>1942</u> , <i>64</i> , 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. <i>J. Am. Chem. Soc.</i> <u>1940</u> , <i>62</i> , 3086.								

COMPONENTS: (1) Triphenylene; $C_{18}H_{12}$; [217-59-4] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Klevens, H.B. <i>J. Phys. Chem.</i> <u>1950</u> , <i>54</i> , 283-98.
VARIABLES: Temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of triphenylene in water at 25°C was reported to be $4.3 \times 10^{-5} \text{ g(1) L}^{-1}$ sln and $1.88 \times 10^{-7} \text{ mol(1) L}^{-1}$ sln. Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $4.28 \times 10^{-6} \text{ g(1)/100 g sln}$ and 3.39×10^{-9} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: (1) Triphenylene; $C_{18}H_{12}$; [217-59-4] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.Y. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 399-402.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of triphenylene in water at 25°C was reported to be 0.043 mg(1) dm^{-3} sln and $x_1 = 3.39 \times 10^{-9}$. The corresponding mass percent calculated by the compiler is 4.3×10^{-6} g(1)/100 g sln.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.	SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. ESTIMATED ERROR: soly. ± 0.00017 mg(1) dm^{-3} sln (maximum deviation from several determinations). REFERENCES: