COMPONENTS:	EVALUATOR:
(1) Propylbenzene, C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION:

Quantitative solubility data for propylbenzene (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 propylbenzene.

TABLE 1: Quantitative Solubility Studies of Propylbenzene (1) in Water (2)

Reference	T/K	Method
Führer (ref 1)	288	volumetric
Stearns *et al.* (ref 2)	298	turbidimetric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Guseva and Parnov (ref 5)	359-495	synthetic
Krasnoshchekova and Gubergrits (ref 7)	298	GLC
Sanemasa *et al.* (ref 8)	288-318	spectrophotometric
Sanemasa *et al.* (ref 9)	298	spectrophotometric

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

Guseva and Parnov (ref 5) have reported solubility data for propylbenzene in water at elevated temperatures (359-495K) and system pressure. Alwani and Schneider (ref 6) have studied phase equilibria in the propylbenzene - water system at 600-678K and 20-200 MPa. In the absence of confirmatory studies no Critical Evaluation of these data is possible; however, it may be noted that data reported by Guseva and Parnov (ref 5) for other hydrocarbon - water systems are generally not reliable. The interested user is referred to the relevant Data Sheets for experimental results.

All other data for the solubility of propylbenzene in water are summarized in Table 2 except for the 298K data of Führer (ref 1) and Klevens (ref 4) which are very much higher than all other studies (ref 3,7,8,9) and are rejected. The remaining data at 298K, the only temperature where comparison is possible, are in only fair agreement.

At other temperatures only the values of Sanemasa *et al.* (ref 8) are available. Thus all solubility values in Table 2 must be considered Tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propylbenzene; C_9H_{12}; [103-65-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	March 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of Propylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values $10^3 g(1)/100g$ sln	"Best" values ($\pm \sigma_n$)[a] $10^3 g(1)/100g$ sln	$10^6 x_1$
288	4.66 (ref 8)	4.7	7.0
298	5.5 (ref 3), 7.0 (ref 7) 5.10 (ref 8), 4.52 (ref 9)	5.5 ± 0.9	8.2
308	5.50 (ref 8)	5.5	8.2
318	6.41 (ref 8)	6.4	9.6

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

REFERENCES

1. Fuhner, H. *Chem. Ber.* 1924, *57*, 510-4.
2. Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, L.D. *J. Chem. Phys.* 1947, *15*, 496-507.
3. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
4. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
5. Guseva, A.N.; Parnov, E.I. *Zh. Fiz. Khim.* 1964, *38*, 805-6.
6. Alwani, Z.; Schneider, G.M. *Ber. Bunsenges. Phys. Chem.* 1969, *73*, 294-301.
7. Krasnoshchekova, R.Y.; Gubergrits, M.Y. *Vodnye. Resursy.* 1975, *2*, 170-3.
8. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, J. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.
9. Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* 1984, *57*, 1539-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Fuhner, H. *Ber. Dtsch. Chem. Ges.* 1924, *57*, 510-5.
VARIABLES:	**PREPARED BY:**
One temperature: 15°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 15°C was reported to be 0.006 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 9×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 cm^3 (2) until a completely clear solution was no longer obtained at the experimental temperature.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; commercial grade; used as received,

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D. *J. Chem. Phys.* 1947, *15*, 496-507.
VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and D. Shaw

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.012 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compiler is 1.8×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Mixtures of (1) in (2) of known composition were shaken for at least 48 hours. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: temp. ± 3°C.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.0055 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 8.2×10^{-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. best grade; fractionally distilled; b.p. range 157.8-158.1°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.12 g(1) L^{-1} sln and 0.001 mol(1) L^{-1} sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1]	Guseva, A.N.; Parnov, E.I.
(2) Water; H_2O; [7732-18-5]	*Zh. Fiz. Khim.* 1964, *38*, 805-6.
VARIABLES:	**PREPARED BY:**
Temperature: 85.8-222.0°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of propylbenzene in water

t/°C	g(1)/100 g sln	$10^5 x_1$ (compiler)
85.8	0.0132	1.98
114.5	0.0166	2.49
140.5	0.0321	4.81
188.0	0.087	13.04
222.0	0.245	36.8

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Vodnye. Resursy.* 1975, *2*, 170-3.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.070 mg(1) cm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0070 g(1)/100 g sln and 1.05×10^{-5}. The assumption that 1.00 cm^{-3} sln = 1.00 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.	(1) described in ref (1). (2) distilled.
	ESTIMATED ERROR: temp. ± 1°C
	REFERENCES: 1. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.
VARIABLES:	PREPARED BY:
Temperature: 15-45°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water

t /°C	10^4 mol(1)/dm^3 sln	10^3 g(1)/100 g sln (compiler)[a]	10^6 x_1 (compiler)[a]
15	3.88 ± 0.15	4.66	6.99
25	4.23 ± 0.12	5.10	7.64
35	4.55 ± 0.07	5.50	8.25
45	5.28 ± 0.17	6.41	9.61

[a] Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

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. ± 0.1°C.

REFERENCES:

1. Kell, G.S.
J. Chem. Eng. Data 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H.
Chem. Lett. 1981, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* 1984, *57*, 1539-44.
VARIABLES: One Temperature: 25°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 3.76×10^{-4} mol(1)/dm^3 sln. Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of 4.52×10^{-3} g(1)/100 g sln, $x_1 = 6.78 \times 10^{-6}$, calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectrophotometry.	(1) Analytical reagent grade source and purity not stated, used without further purification. (2) Deionized and redistilled; no further details given.
	ESTIMATED ERROR: Not specified.
	REFERENCES: 1. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.