COMPONENTS:	EVALUATOR:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985

CRITICAL EVALUATION:

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

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

REFERENCE	T/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	residue volume
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 3)	391-484	(1) in (2)	unspecified
Englin et al. (ref 4)	293-313	(2) in (1)	analytical
Sutton and Calder (ref 5)	298	(1) in (2)	GLC
Sanemasa et al. (ref 6)	288-318	(1) in (2)	spectrophotometric
Sanemasa et al. (ref 7)	288-318	(1) in (2)	spectrophotometric

The original data in 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.   THE SOLUBILITY OF MESITYLENE (1) IN WATER (2)

All the available data on the solubility of mesitylene in water at low temperatures (288-318K) are summarized in Table 2, except for the rejected values referred to below.

At 298K, the only temperature where comparison is possible, the datum of Sutton and Calder (ref 5) is in good agreement with the values reported by Sanemasa et al. (ref 6,7) enabling the mean to be Recommended. The datum of Andrews and Keefer (ref 2) is markedly higher than the other studies (ref 5,6,7) and is rejected as is the approximate value of Booth and Everson (ref 1).

At other temperatures only the two data sets of Sanemasa et al. (ref 6,7) are available and must thus be considered as Tentative.

At the elevated temperatures (ca. 390-480K) and system pressure only the data of Guseva and Parnov (ref 3) are available and thus no Critical Evaluation is possible. However, it may be noted that solubilities reported by Guseva and Parnov are not always reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

COMPONENTS:	EVALUATOR:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985.

CRITICAL EVALUATION: (continued)

TABLE 2:   Recommended (R) and Tentative Values of the Solubility of Mesitylene (1) in Water (2)

T/K	Reported values 10^3g(1)/100g sln	"Best" values ($\pm \sigma_n$) 10^3g(1)/100g sln	$10^6 x_1$
288	4.56 (ref 6), 4.60 (ref 7)	4.6	6.9
298	4.82 (ref 5), 4.95 (ref 6) 5.00 (ref 7)	4.89 ± 0.08^a (R)	7.4 (R)
308	5.42 (ref 6), 5.49 (ref 7)	5.4	8.2
318	5.65 (ref 6), 5.89 (ref 7)	5.7	8.7

a Obtained by simple averaging; σ_n has no statistical significance.

2.   THE SOLUBILITY OF WATER (2) IN MESITYLENE (1)

The solubility of water in mesitylene has been reported only by Englin *et al.* (ref 4) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for experimental values. However, it may be noted that for other hydrocarbon systems studies by Englin *et al.* their results are generally reliable at $T < 300K$ but are higher than Recommended values at higher temperatures.

REFERENCES

1.   Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* <u>1948</u>, *40*, 1491-3.

2.   Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* <u>1950</u>, *72*, 5034-7.

3.   Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1963</u>, *18*, 76-9.

4.   Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Khim. Tekhnol. Topl. Masel* <u>1965</u>, *10*, 42-6.

5.   Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* <u>1975</u>, *20*, 320-2.

6.   Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Chem. Lett.* <u>1981</u>, 225-8.

7.   Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* <u>1982</u>, *55*, 1054-62.

8.   Alwani, Z.; Schneider, G.M. *Ber. Bunsenges. Phys. Chem.* <u>1969</u>, *73*, 294-301.

NOTE ADDED IN PROOF

Alwani and Schneider (ref 8) have also reported a critical locus of the mesitylene-water system.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* <u>1948</u>, *40*, 1491-3.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of mesitylene in water at 25°C
was reported to be less than 0.02 g(1)/100 mL (2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

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.	(1) source not specified;
	    CP or highest commercial
	    grade; used as received.
	
	(2) distilled.

	ESTIMATED ERROR: soly. ± 0.1 mL(1)/100 mL(2).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C_9H_{12}; [108-67-8] (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 mesitylene in water at 25°C was reported
to be 0.0097 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers
is 1.45×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 spectrophoto-meter.	(1) Eastman Kodak Co. white label; fractionally distilled; b.p. 165.0°C. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1963</u>, *18*, 76-9.
VARIABLES: Temperature: 118-211°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of mesitylene in water

$t/°C$	g(1)/100 g sln	$10^4 x_1$ (compiler)
118	0.007	0.10
144	0.013	0.19
187	0.041	0.61
211	0.078	1.17

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made in sealed glass tubes. No details were reported in the paper.	(1) source not specified; n_D^{20} 1.49945. (2) doubly distilled.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water· H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.

VARIABLES:	PREPARED BY:
Temperature: 20-40°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in Mestitylene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
20	0.0291	1.94
30	0.0393	2.62
40	0.0519	3.45

AUXILIARY INFORMATION

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of mesitylene in water at 25°C was reported to be 48.2 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00482 g(1)/100 g sln and 7.22×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma-tography.	(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 0.1°C soly. 0.3 (the standard deviation of the mean for six replicates).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Chem. Lett.* <u>1981</u>, 225-8.
VARIABLES: Temperature: 15-45°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of mesitylene in water

$t/°C$	$g(1)/L$	$g(1)/100 \text{ g sln}$[a]	$10^6 x_1$[a]
15	0.0456 ± 0.0010	0.00456	6.82
25	0.0495 ± 0.0015	0.00495	7.41
35	0.0542 ± 0.0033	0.00542	8.11
45	0.0565 ± 0.0031	0.00565	8.46

[a]calculated by compiler assuming a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, generated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous sln were transferred into funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported. The solubility runs were made such that the temperature of solute reservoir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.	(1) analytical reagent grade used as purchased. (2) redistilled. ESTIMATED ERROR: soly. : given above REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene (1,3,5-Trimethyl-benzene); C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* <u>1982</u>, *55*, 1054-62.
VARIABLES: Temperature: 15-45°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of 1,3,5-trimethylbenzene 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	3.83 ± 0.15	4.60	6.90
25	4.15 ± 0.22	5.00	7.50
35	4.55 ± 0.23	5.49	8.22
45	4.85 ± 0.32	5.89	8.83

[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.), stated purity 97.0%, 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 <u>1975</u>, *20*, 97.

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene (1,3,5-Trimethyl-benzene); C_9H_{12}; [108-67-8] (2) Artificial seawater (ref 1)	Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* <u>1975</u>, *20*, 320-2.
VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	PREPARED BY: M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of 1,3,5-trimethylbenzene in artificial seawater is reported to be 31.3 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 3.13 x 10^{-3} g(1)/100 g sln and 4.81 x 10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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. ± 0.1°C

soly. 0.2 (std. dev.)

REFERENCES:
1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* <u>1940</u>, *3*, 135.