COMPONENTS:	EVALUATOR:
(1) 1,4-Difluorobenzene; $C_6H_4F_2$; [540-36-3]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979.

CRITICAL EVALUATION:

Two experimental measurements have been reported on the solubility of 1,4-difluorobenzene in water (1,2). Jockers (1) has determined the solubility at high temperatures between 533 K and 553 K and high pressures only in connection with studies of the parameters that influence phase separation. The single solubility measurement reported by Yalkowsky et al. (2) cannot be easily compared with the results of Jockers. Both results are included in the table below.

According to the authors (3), the accuracy of the experimental determinations reported by Yalkowsky et al. was ± 10 percent. This is a reasonable observation considering the details available on the experimental procedure. The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1,4-difluorobenzene in water is tentative:

$P/P_\theta = 1.0$

T/K	10^2mol(1)/dm^3	g(1)/kg	$10^4 x$(1)
298.15	1.07	1.22	1.94

$P/P_\theta = 80 - 100 \times 10^5$

T/K	mol(1)/dm^3	10^{-2}g(1)/kg	$10^2 x$(1)
533.15-553.15	3.47	3.50	7.84

REFERENCES

1. Jockers, R., Ph.D. Dissertation, University of Bochum, Bochum, 1976.

2. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

3. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Difluorobenzene; $C_6H_4F_2$; [540-36-3] (2) Water; H_2O; [7732-18-5]	Jockers, R., Ph.D. Dissertation, University of Bochum, Bochum, 1976, pp 94-5.
VARIABLES:	PREPARED BY:
Temperature and pressure	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	P/bar	10^{-2}g(1)/kg [a]	mol(1)/kg [b]	10^2x(1) [c]
260.0	80	3.501	3.069	7.84
270.0	92	3.501	3.069	7.84
280.0	100	3.501	3.069	7.84

a. Calculated by compiler.
b. Calculated by F. W. Getzen.
c. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made using a high temperature, high pressure optical cell made from stainless steel with an internal stirrer. Predetermined mixtures of 1,4-difluorobenzene in water were introduced into the cell and homogenized at various temperatures and pressures. The phase transitions were observed through a sapphire window at the appropriate temperatures and pressures. Further details have been included in (1,2).

SOURCE AND PURITY OF MATERIALS:

$C_6H_4F_2$: Fluka AG., Buchs, Schweiz, 99.5% pure, redistilled before use.

H_2O: Boiled with $KMnO_4$ and redistilled before use.

ESTIMATED ERROR:

Solubility: ±1%.
Temperature: ±0.5 K.
Pressure: ±2 bar.

REFERENCES:

1. Götze, G.; Jockers, R.; Schneider, G. M. 4th Inter. Conf. Chem. Thermodyn. IUPAC, Montpellier, Aug. 26-30, 1975, Part IV/9, pp 57-64.
2. Jockers, R.; Schneider, G. M. *Ber. Bunsenges. Phys. Chem.* 1978, *83*, 576-62.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Difluorobenzene; $C_6H_4F_2$; [540-36-3] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	g(1)/dm^3 [a]	10^2mol(1)/dm^3 [b]	$10^4 x$(1) [c]
25	1.221	1.07	1.935

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A small excess of 1,4-difluorobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The filtrate was diluted and assayed spectrophotometrically. The determination was done in duplicate.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4F_2$: Aldrich commercial grade, used as received.

H_2O: Deionized.

ESTIMATED ERROR:

Solubility: ±10%.

Temperature: ±1 K.

REFERENCES: