COMPONENTS:	EVALUATOR:
(1) 1-Chloro-2-iodobenzene; C_6H_4ClI; [615-41-8]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979

CRITICAL EVALUATION:

The experimental results consist of a single value at 298.15 K published by 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations 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-chloro-2-iodobenzene in water is tentative:

T/K	10^4mol(1)/dm^3	10^2g(1)/kg	$10^6 x$(1)
298.15	2.88	6.89	5.21

REFERENCES

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

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Chloro-2-iodobenzene; C_6H_4ClI; [615-41-8] (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	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	6.868	2.88	5.204

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A small excess of 1-chloro-2-iodobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometrically. Two independent determinations were carried out.

SOURCE AND PURITY OF MATERIALS:

C_6H_4ClI: Aldrich commerical grade, used as received.

H_2O: Deionized.

ESTIMATED ERROR:
Solubility: ±10%.

Temperature: ±1 K.

REFERENCES: