COMPONENTS:	EVALUATOR:
(1) 4-Bromophenol; C_6H_5BrO; [106-41-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

The only two available reported measurements of the solubility of 4-bromophenol in water were published many years apart and the information concerning the methods of analysis provided in the earlier of these works is incomplete. The older one by Werner (1) appeared in 1884 and the other more recent work was published in 1971. Therefore, certain difficulties have been encountered in the evaluation of these combined data. The solubility measurements reported by Parsons, Rochester, and Wood (2) for 4-bromophenol in water appear quite reliable when the saturation equilibrium, the method of analysis, and the reported standard deviation have been considered. On the basis of these criteria, the value reported by Werner should be rejected. However, if one can accept a satisfactory state of purity for the synthesized material, the value of Werner, which refers to a temperature of 288 K, can be regarded as fairly good. Considering the difference in the temperatures of the reported solubility values, the agreement between the two values is quite satisfactory in spite of the long time interval between their determinations. However, the solubility value reported by Parsons et al. must be considered as only a tentative value.

It should be noted that the solubility of 4-bromophenol in water is considerably dependent upon the acidity of the solution. Here, it is assumed that the solubility established refers to that of a solution having a pH value prevailing for saturated 4-bromophenol in water. An entire series of measurements of solubilities at various pH values is required to complete the picture of the solubility behavior for protolyzing compounds such as 4-bromophenol in water.

The solubility of 4-bromophenol in water is reported here as a tentative value:

T/K	$10 mol(1)/dm^3$	$10^{-1} g(1)/kg$	$10^3 x(1)$
298.15	1.07	1.86	1.97

REFERENCES

1. Werner, E. *Ann. Chim. Phys. Series 6(III)* 1884, 567-74.

2. Parsons, G. H.; Rochester, C. H.; Wood, C.E.C. *J. Chem. Soc. B* 1971, 533-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Bromophenol; C_6H_5BrO; [106-41-2] (2) Water; H_2O; [7732-18-5]	Werner, E. *Ann. Chim. Phys. Series 6(III)* 1884, 567-74.
VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

t/°C	10^{-1}g(1)/dm^3 [a]	10^2mol(1)/dm^3 [b]	10^3x(1) [b]
15	1.42	8.207	1.499

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Information about the saturation process was incomplete. The analysis of the saturated solution was done using titrimetry with bromine.	C_6H_5BrO: Synthesized product, melting point 64°C, boiling point 137°C at 28 mm Hg pressure. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Bromophenol; C_6H_5BrO; [106-41-2] (2) Water; H_2O; [7732-18-5]	Parsons, G. H.; Rochester, C. H.; Wood, C. E. C. *J. Chem. Soc. B* 1971, 533-6.
VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

t/°C	10^{-1}g(1)/kg [a]	10mol(1)/kg(2) [b]	$10^3 x$(1) [a]
25	1.8261	1.075	1.9330

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental procedure was probably similar to that reported in (1). Excess solid was shaken with water at 25 ± 0.1°C for 24 hours. The saturated solution was then filtered at thermostat temperature and, with appropriate dilution, analyzed spectrophotometrically. Linear calibration graphs of absorbance at a wave length of maximum absorbance of the neutral phenols against concentration confirmed the applicability of the Beer-Lambert law for the analyses.

SOURCE AND PURITY OF MATERIALS:

C_6H_5BrO: Commercial product (manufacturer not reported), recrystallized to a constant melting point.

H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: ±2% (standard deviation of the average value from five determinations as reported by the authors).

REFERENCES:

1. Parsons, G. H.; Rochester, C. H.; Rostron, A.; Sykes, P. C. *J. Chem. Soc. Perkin Trans. II(1)* 1972, 136-8.