Chapter 15

SOLUBILITY IN WATER AND OCTANOL-WATER PARTITION COEFFICIENT

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ABSTRACT

Results for water solubility and octanol-water partition coefficient are presented for major organic chemicals. The results are provided in an easy-to-use table that is especially applicable for rapid engineering usage with the personal computer or hand calculator. Typical water solubility values are 786 ppm(wt) for carbon tetrachloride (CCl4) and 0.002 ppm(wt) for tetradecane (C14H30).

INTRODUCTION

Physical and thermodynamic property data for organic chemicals are of special value to engineers in the chemical processing and petroleum refining industries. In this article results are presented for water solubility and octanol-water partition coefficient. The compilation of data is intended for use in engineering and environmental studies. As an example of such usage, solubility data are useful in determining the assessment and distribution of a chemical spill upon its contact with water.

SOLUBILITY IN WATER

The results for solubility of organic compounds in water are given in Table 15-1. The presented values are applicable to a wide variety of substances including alkanes, olefins, diolefins, alkynes, cycloalkanes, aromatics, fluorocarbons, chlorocarbons, bromocarbons, iodocarbons, alcohols, acids, ketones, aldehydes, ethers, esters, amines, nitriles, sulfides and thiols. The tabulation also gives the molecular weight, freezing point and normal boiling point. The last two columns provide the data for solubility in water on a weight and mole basis. The compilation is based on both experimental and estimated values.

The tabulation is arranged by carbon number (C, C2, C3, ... C28) to provide ease of use in quickly locating solubility data using the chemical formula.

For the tabulation, the solubility data for liquids (compounds with boiling point greater than 25 C) apply for the aqueous liquid phase in contact with a vapor which contains the compound, water and air. The solubility data for gases (compounds with boiling point less than 25 C) apply for the aqueous liquid phase in contact with a vapor which contains only the compound and water.

In preparing the compilation, a literature search was conducted to identify data source publications (1-190). Both experimental values for the property under consideration and parameter values for estimation of the property are included in the source publications. The publications were screened and copies of appropriate data were made. These data were then keyed-in to the computer to provide a database of solubility values for organic compounds for which experimental data are available. The database also served as a basis to check the accuracy of the estimation method.

Upon completion of data collection, estimation of solubility for compounds was performed using the boiling point correlation developed by Yaws and co-workers (185-190):

$$\log_{10} S = A + BT_B + CT_B^2 + DT_B^3 \qquad (15\text{-}1)$$

where S = solubility in water at 25 C, parts per million by weight, ppm(wt)
T_B = boiling point temperature of compound, K
A, B, C and D = regression coefficients for chemical family

Results from the correlation are in favorable agreement with experimental data for solubility in water.

Estimation of solubility for hydrocarbons and organic oxygen compounds was accomplished using the following regression coefficients:

<u>alkanes (paraffins)</u>

A = -17.652 (normal and isomers)
B = 177.811E-03
C = -500.907E-06
D = 411.124E-09

<u>cycloalkanes (naphthenes)</u>

A = -16.7 for cyclohexanes
A = -16.9 for cyclopentanes
B = 177.811E-03
C = -500.907E-06
D = 411.124E-09

<u>benzenes (aromatics)</u>

A = -24.008 (no and single substitutions)

<u>alcohols</u>

A = 45.6398 (normal and isomers)

A = -23.650 (double and triple substitutions)
B = 221.196E-03
C = -555.632E-06
D = 418.830E-09

B = -2.3859E-01
C = 4.8739E-04
D = -3.7160E-07

ketones

A = 45.223 (normal and isomers)
B = -2.3859E-01
C = 4.8739E-04
D = -3.7160E-07

ethers

A = 7.510 (normal and isomers)
B = 3.2057E-03
C = -4.0887E-05
D = 4.7284E-09

aldehydes

A = 20.4898 (normal and isomers)
B = -9.0310E-02
C = 1.9223E-04
D = -1.7856E-07

This correlation is applicable to substances that are liquids at ambient conditions (25 C, 1 atm). For hydrocarbons (alkanes, cycloalkanes and benzenes), the range for boiling point temperatures is 298 to 561 K. For organic oxygen compounds (alcohols, ketones, ethers and aldehydes), the range for boiling point temperatures is 298 to 625 K. The correlation is not applicable to solids since a different solubility curve is obtained for solids.

Estimation of solubility for the remaining compounds (olefins, diolefins, alkynes, sulfides, thiols and esters) was also accomplished using a modified boiling point method. Due to the small database, the estimates for these compounds should be considered rough approximations. The estimates for hydrocarbons and organic oxygen compounds are more accurate.

A comparison of experimental and estimated data values for solubility in water is shown in Figure 15-1 for paraffins, naphthenes and aromatics. The graph discloses favorable agreement of experimental and estimated values.

OCTANOL-WATER PARTITION COEFFICIENT

The octanol-water partition coefficient is the ratio of a chemicals concentration in an octanol phase to its concentration in an aqueous phase:

Kow = (concentration in octanol phase) / (concentration in aqueous phase) (15-2)

The results for octanol-water partition coefficient are also given in Table 15-1. Both experimental and estimated values are provided in the compilation that is based on data source publications for organic compounds (1-60). Many of the estimates are based on the atom-fragment contribution method as described by Meylan and Howard. (57). The tabulation is arranged by chemical formula to provide ease of use in quickly locating data.

Properties such as octanol-water partition coefficient (Kow) are useful in studies involving the environmental fate of chemicals. As an example of such usefulness in environmental applications, Lyman, Reehl and Rosenblatt (42) discuss how water solubility, soil-sediment coefficient and biological concentrations for aquatic life can be related to Kow. Chemicals with low Kow values tend to have high solubilities in water, low soil-sediment coefficients and small biological concentrations for aquatic life.

EXAMPLES

The tabulation and correlation maybe used for determining solubility of organic compounds in water. Examples are shown below.

Example 1 A chemical spill of carbon tetrachloride (CCl4) occurs into a body of water at ambient conditions (25 C, 1 atm). Determine the concentration of carbon tetrachloride in the water.

Using the chemical formula (CCl4) for carbon tetrachloride, inspection of the table discloses that the solubility in water is:

S = 785.7 ppm(wt)

Example 2 A chemical spill of ethylbenzene (C8H10) occurs into a body of water at ambient conditions (25 C, 1 atm). Determine the concentration of ethylbenzene in the water.

Using the chemical formula (C8H10) for ethylbenzene, inspection of the table discloses that the solubility in water is:

S = 165.1 ppm(wt)

Example 3 Estimate the solubility of pentane (C5H12) in water at a temperature of 298.15 K (25 C).

Substitution of the regression coefficients (A, B, C and D) and boiling temperature (309.22 K) into the equation for solubility of paraffins (alkanes) in water yields:

$$\log_{10} S = -17.652 + 177.811E\text{-}03 * 309.22 - 500.907E\text{-}06 * 309.22^2 + 411.124E\text{-}09 * 309.22^3 = 1.59106$$

$$S = 10^{1.59106}$$

S = 39.00 ppm(wt)

The calculated and data values compare favorably (39.00 Vs 38.50, deviation = 0.50/38.50 = 1.3%).

Portions of this material appeared in Chem. Eng., 97, 177 (April,1990), Chem. Eng., 97, 115 (July, 90), Pollution Engineering, 22, 70 (Oct., 1990), Oil & Gas Journal, 89, 79 (April 8, 1991), Oil & Gas Journal, 89, 86 (Sept. 16, 1991) and Oil & Gas Journal, 95 (35), 80 (Aug. 29, 1994). These portions are reprinted by special permission.

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