Chapter 18

HENRY'S LAW CONSTANT FOR COMPOUND IN WATER

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ABSTRACT

Results for Henry's law constant are presented for a wide variety of organic chemicals in water. The organic chemicals include hydrocarbon, oxygen, nitrogen, fluorine, chlorine, bromine, iodine and sulfur compounds. 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. Representative values for Henry's law constant (atm/mol fraction) are 11,515 for ethylene (C2H4), 1,630 for carbon tetrachloride (CCl4) and 308 for benzene (C6H6) at ambient conditions.

INTRODUCTION

Physical and thermodynamic property data for major organic chemicals are of special value to engineers in the chemical processing and petroleum refining industries. In this article results are presented for Henry's law constant for organic chemicals in water. The compilation is intended for use in initial engineering and environmental impact studies. As an example of such usage, Henry's law constant is helpful in determining the environmental movement and fate of chemicals in air and water.

The results are presented in an easy-to-use tabular format that is especially applicable for rapid engineering usage with the personal computer or hand calculator.

HENRY'S LAW CONSTANT

The results for Henry's law constant for organic chemicals in water are given in Table 18-1. The tabulation is applicable to a wide variety of organic chemicals in contact with water at ambient conditions. The wide variety of substances includes hydrocarbons, fluorocarbons, chlorocarbons, bromocarbons, iodocarbons, alcohols, acids, ketones, aldehydes, ethers, esters, amines, nitriles, sulfides and thiols.

The tabulation is arranged by carbon number (C1, C2, C3, ... C28). This provides ease of use in quickly locating data using the chemical formula.

Henry's law constant may be determined from data for solubility, vapor pressure, and activity coefficient at infinite dilution (see Appendix for equations). Thus, in preparing the tabulation, a literature search was conducted to identify data source publications (1-210) for solubility, vapor pressure, activity coefficient at infinite dilution, and Henry's law constant. 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.

A comparison of calculated and data (experimental) values for Henry's law constant is shown in Figures 18-1 and 18-2. The graph in Figure 18-1 includes many different organic chemicals (carbon monoxide; carbon dioxide; trichlorofluoromethane; carbon tetrachloride; bromoform; chloroform; dichloromethane; trichlorotrifluoroethane; tetrachloroethylene; hexachloroethane; trichloroethylene; 1,1-dichloroethylene; cis 1,2-dichloroethylene, trans 1,2-dichloroethylene; 1,1,2,2-tetrachloroethane; vinyl chloride; 1,1,1-trichloroethane; 1,1,2-trichloroethane; 1,2-dibromoethane; 1,1-dichloroethane; ethyl chloride; 1,2,3-trichloropropane; 1,2-dichloropropane; 1,3-dichloropropane; 1-chlorobutane; 2-chlorobutane; 1-chloropentane; 1,2,4-trichlorobenzene; 1,3-dichlorobenzene; 1,2-dichlorobenzene; chlorobenzene and nitrobenzene) which contain a variety of functional groups. The graph discloses general agreement of calculated and data values for the different organic chemicals.

The graph in Figure 18-2 includes many different types of hydrocarbons (alkane, olefin, acetylinic, naphthenic and aromatic hydrocarbons: methane, ethane, hexane, 2-methylpentane, 2-methylhexane; heptane; octane; ethylene, acetylene, cyclopentane; cyclohexane, methyl cyclohexane; benzene, toluene, o-xylene, m-xylene, p-xylene, ethyl benzene, propyl benzene, cumene, 1,3,5-trimethylbenzene; 1,2,4-trimethylbenzene; tetralin and 1-methylnaphthalene). The graph discloses general agreement of calculated and data values for the different hydrocarbon types.

The compilation for Henry's law constant is usable for engineering and environmental impact studies involving organic compounds in water.

EXAMPLES

The tabulation maybe used for determining Henry's law constant for the compound in water. The use of Henry's law constant in environmental applications is illustrated below.

Example 1 A chemical spill of ethylbenzene (C8H10) occurs into a body of water. The concentration of ethylbenzene in the liquid at the surface of the water is 25 parts per million on a mol basis (x_i = 25 ppm(mol)). Estimate the concentration of ethylbenzene in the air at the surface of the water.

From thermodynamics at low pressure, the partition coefficient is given by $K_I=H_i/P_t$. Substitution of Henry's law constant (H_i = 452.3 atm/mol fraction for ethylbenzene) from the table and the total pressure (P_t = 1 atm) into this equation provides K_i = 452.3/1 = 452.3.

Since the vapor concentration is given by $y_i = K_i * x_I$, substitution of the K value (K_i = 452.3) and liquid concentration (x_i = 25 ppm) yields:

$$y_i = K_i * x_i = 452.3 * 25$$

$$y_i = 11{,}308 \text{ ppm (mol)}$$

Example 2 A chemical spill of benzene (C6H6) occurs into a body of water. The concentration of benzene in the air at the surface of the water is measured at 1000 parts per million on a mol basis (y_i = 1000 ppm(mol)). Estimate the concentration of benzene in the liquid at the surface of the water.

From thermodynamics at low pressure, the partition coefficient is given by $K_i = H_i/P_t$. Substitution of Henry's law constant (H_i = 308.26 atm/mol fraction for benzene) from the table and the total pressure (P_t = 1 atm) into the above equation provides K_i = 308.26/1 = 308.26.

Since the liquid concentration is given by $x_i = y_i / K_I$, substitution of the K value (K_i = 308.26) and vapor concentration (y_i = 1000 ppm) yields:

$$x_i = y_i / K_i = 1000/308.26$$

$$x_i = 3.24 \text{ ppm (mol)}$$

Portions of this material appeared in Chem. Eng., 98, 179 (Nov., 1991). These portions are reprinted by special permission.

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1-190. See **REFERENCES – WATER SOLUBILITY - ORGANIC COMPOUNDS** in **Chapter 15 SOLUBILITY IN WATER AND OCTANOL-WATER PARTITION COEFFICIENT**

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