

Chapter 7

VAPOR PRESSURE

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ABSTRACT

Results for vapor pressure as a function of temperature are presented for major organic and inorganic chemicals. The coefficients in the equation for vapor pressure are displayed in easy-to-use tabulations that are especially applicable for rapid engineering usage with the personal computer or hand calculator. The chemicals encompass many compound types.

INTRODUCTION

Physical and thermodynamic property data such as vapor pressure are of special value to engineers in the chemical processing and petroleum refining industries. As an example, knowledge of the vapor pressure of the compound is required in the design of a storage vessel to contain the compound. In hazard analysis and vent system technology, vapor pressure at the specified temperature is important. In vapor-liquid operations, such as distillation, knowledge of vapor pressure (and activity coefficients) is required for determining K-values. In this article, results for vapor pressure as a function of temperature are presented.

VAPOR PRESSURE CORRELATION

The Antoine-type equation with extended terms was selected for correlation of vapor pressure as a function of temperature:

$$\log_{10} P = A + B/T + C \log_{10} T + D T + E T^2 \quad (7-1)$$

1)

where

P = vapor pressure, mm Hg

A,B,C,D and E = regression coefficients for chemical compound

T = temperature, K

The results for vapor pressure are given in Tables 7-1 and 7-2. The temperature range for which the equation may be used to predict vapor pressure is denoted by the respective minimum and maximum temperatures (TMIN and TMAX).

The tabulation for organic compounds is applicable to a wide variety of substances: hydrocarbons (alkanes, olefins, acetylenes, cycloalkanes, aromatics,); oxygenates (alcohols, aldehydes, ketones, acids, ethers, glycols, anhydrides,); halogenates (chlorinated, brominated, fluorinated and iodinated compounds); nitrogenates (nitriles, amines, cyanates, amides,); sulfur compounds (mercaptans, sulfides, sulfates,); silicon compounds (silanes, chlorosilanes,) and many other types.

The tabulation for inorganic compounds provides coverage for a wide range of substances: carbon oxides (carbon monoxide, carbon dioxide,...); nitrogen oxides (nitric oxide, nitrous oxide,...); sulfur oxides (sulfur dioxide, sulfur trioxide,...); hydrogen oxides (water, hydrogen peroxide,...); ammonias (ammonia, ammonium hydroxide,...); hydrogen halides (hydrogen chloride, hydrogen fluoride,...); sulfur acids (sulfuric acid, hydrogen sulfide,...); hydroxides (sodium hydroxide, potassium hydroxide,...); silicon halides (trichlorosilane, silicon tetrachloride,...); ureas (urea, thiourea,...); cyanides (hydrogen cyanide, cyanogen chloride,...); hydrides (silane, diborane,...); sodium derivatives (sodium chloride, sodium fluoride,...); aluminum derivatives (aluminum borohydride, aluminum fluoride,...) and many other compound types. Many elements (total = 82) are covered: hydrogen, nitrogen, oxygen, helium, argon, neon, chlorine, bromine, iodine, fluorine, sulfur, phosphorous, aluminum, lead, tin, mercury, sodium, magnesium, silicon, antimony, boron, iron, chromium, cobalt, titanium, tantalum, silver, gold, platinum, radon, uranium and many others.

In preparing the compilation, a literature search was conducted to identify data source publications for organics (1-41) and inorganics (1-61). 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 for appropriate data. The compilation resulting from the screening is based on both experimental data and estimated values. In the absence of experimental data, estimates were primarily based on Riedel equation (29) and on adjusting the A value in the equation to match the boiling point temperature of the compound. The estimates of the other coefficients for the compound were based on the same values of the compound's brother (closest member of same chemical family). Experimental data and estimates were then regressed to provide the same equation for all compounds.

A comparison of calculated values and experimental data for vapor pressure is shown in Figure 7-1 for a representative chemical. The graph indicates good agreement of calculations and data.

EXAMPLES

The tabulated values maybe used for prediction and calculation of vapor pressure. Examples are given below.

Example 1 Estimate the vapor pressure of methanol (CH₄O) at a temperature of 25.13 C (298.28 K).

Substitution of the coefficients from the table and temperature into the equation for vapor pressure yields:

$$\log_{10} P = 45.6171 - 3.2447E+03/298.28 - 1.3988E+01 \cdot \log_{10}(298.28) + 6.6365E-03 \cdot 298.28 - 1.0507E-13 \cdot 298.28^2 = 2.1034$$

$$P = 10^{2.1034}$$

$$P = 126.88 \text{ mm Hg}$$

The calculated and data values compare favorably (126.88 vs 127.90, deviation = 0.80%).

Example 2 Estimate the vapor pressure of acetone (C₃H₆O) at a temperature of 47.35 C (320.50 K).

Substitution of the coefficients from the table and temperature into the equation for vapor pressure yields:

$$\log_{10} P = 28.5884 - 2.4690E+03/320.50 - 7.3510E+00 \cdot \log_{10}(320.50) + 2.8025E-10 \cdot 320.50 + 2.7361E-06 \cdot 320.50^2 = 2.7456$$

$$P = 10^{2.7456}$$

$$P = 556.71 \text{ mm Hg}$$

The calculated and data values compare favorably (556.71 vs 558.40, deviation = 0.30%).

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