Chapter 1

CRITICAL PROPERTIES AND ACENTRIC FACTOR

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ABSTRACT

Results for critical properties and acentric factor are presented for major organic and inorganic compounds. The critical properties include critical temperature, pressure, volume, density and compressibility factor. The chemical formula, molecular weight, freezing point and boiling point are also given. The results are displayed in easy-to-use tabulations which are especially applicable for rapid engineering usage with the personal computer or hand calculator. The chemicals encompass hydrocarbon, oxygen, nitrogen, halogen, silicon, sulfur and other compound types.

INTRODUCTION

Physical and thermodynamic property data for organic and inorganic chemicals are of special value to engineers in the chemical processing and petroleum refining industries. The engineering design of process equipment often requires knowledge of such properties as heat capacity, enthalpy, density, viscosity, thermal conductivity and others.

In this article, results are presented for critical properties and acentric factor, which are usable in corresponding states correlations to determine properties such as heat capacity, enthalpy, density, viscosity and thermal conductivity. The results are intended for initial engineering studies and are presented in an easy-to-use tabular format which is especially applicable for rapid engineering usage with the personal computer or hand calculator.

CRITICAL PROPERTIES AND ACENTRIC FACTOR

The results for critical properties and acentric factor are shown in Tables 1-1 and 1-2 for organic and inorganic compounds. The tabulations are based on both experimental data and estimated values.

In the data collection, a literature search was conducted to identify data source publications for organics (1-44) and inorganics (1-59). 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 into the computer to provide a database of critical properties for 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 the critical properties and acentric factor for the remaining compounds was performed. For organic compounds, the group contribution method of Joback as given by Reid, Prausnitz and Poling (29) was primarily used for the estimation of critical temperature (T_C), pressure (P_C) and volume (V_C).

For inorganic compounds, estimates of critical temperature were based on modifications of the Guldberg-Guye rule (11), Gates-Thodos method (11) and Grosse equation (11). Estimates of other critical constants and acentric factor were primarily based on extension of the vapor pressure curve and modifications of the Benson relation (11) and Herzog proposal (11). Very limited experimental data for critical constants and acentric factor are available for inorganic compounds and elements that are solids at room temperature. Thus, the estimates for these substances should be considered rough approximations in the absence of experimental data.

Critical density (ρ_C) was determined from dividing molecular weight by critical volume:

$$\rho_C = MW / V_C \qquad (1\text{-}1)$$

where ρ_C = critical density, g/cm^3
MW = molecular weight, g/mol
V_C = critical volume, cm^3/mol

Critical compressibility factor (Z_C) was ascertained from applying the gas law at the critical point:

$$Z_C = P_C V_C / R T_C \qquad (1\text{-}2)$$

For many of the compounds, the acentric factor (ω) was estimated by the following equation which is given in Reid, Prausnitz and Poling (29):

3 T_B / T_C

$$\omega = \frac{7}{1 - T_B / T_C} (\log P_C) - 1 \qquad (1\text{-}3)$$

where ω = acentric factor
T_B = boiling point temperature, K
T_C = critical temperature, K
P_C = critical pressure, atm.

This equation for acentric factor is based on extending the vapor pressure by the Antoine type relation.

Comparisons of estimates and data for critical temperature are shown in Figures 1-1 and 1-2 for normal alkanes and elements. Both graphs disclose favorable agreement of estimates and data.

A comparison of the estimates with experimental data was favorable for the group contribution method of Joback for organic compounds. Average absolute errors of 0.9%, 6.3%, 4.4% and 4.6% were experienced for critical temperature (465 compounds), pressure (453 compounds), volume (345 compounds) and compressibility factor (348 compounds). Average absolute error for acentric factor (277 compounds) was about 6%.

The normal boiling (T_B) and freezing (T_F) point temperatures are also given in the table. For most compounds, data are available. For the compounds without data, the group contribution method of Joback (29) was used to estimate the boiling and freezing point temperatures for organic compounds. As discussed by Reid, Prausnitz and Poling (29), no reliable methods are available for precise estimation of freezing point temperature. Thus, the estimates for freezing point temperature should be considered as rough approximations.

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