Chapter 2

HEAT CAPACITY OF GAS

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ABSTRACT

Results for heat capacity of ideal gas as a function of temperature are presented for major organic and inorganic compounds. The results cover a wide temperature range and include hydrocarbon, oxygen, nitrogen, halogen, sulfur, silicon and many other chemical types. The agreement between correlation and data is quite good.

INTRODUCTION

Thermodynamic properties such as heat capacity are important in the engineering design of chemical processes. In gas-phase chemical reactions, the heat capacity is required to determine the energy (heat) necessary to bring the chemical reactants up to reaction temperature. Additional uses include generalized heat exchanger and energy balance design calculations.

In this article, correlation results for heat capacity of gas are provided in an easy-to-use tabular format that is especially applicable for rapid engineering use with the personal computer or hand calculator.

HEAT CAPACITY CORRELATION

The correlation for heat capacity of the ideal gas is a series expansion in temperature:

$$C_P = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4 \qquad (2\text{-}1)$$

where C_P = heat capacity of ideal gas, joule/(mol K)
A, B, C, D, E = regression coefficients for chemical compound
T = temperature, K

The results for heat capacity of gas are given in Tables 2-1 and 2-2. The tabulations are based on regression of experimental data and estimates from an extensive literature search for organics (1-40) and inorganics (1-78). Both experimental values for the property under consideration and parameter values for estimation of the property are included in the source publications. The numerous data points were processed with a generalized least-squares computer program for minimizing the deviations.

The tabulation for organic compounds is applicable to a wide variety of substances: hydrocarbons (alkanes, olefins, acetylenes, cycloalkanes, ...); 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 chemical types.

The tabulation for inorganic compounds is also comprehensive: 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 bromide, aluminum chloride,...) and many other compound types. Many elements 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 chemical types.

A comparison of correlation and actual data for heat capacity is shown in Figure 2-1 for a representative chemical. The graph indicates good agreement of correlation and data.

EXAMPLES

The correlation results maybe used for prediction and calculation of heat capacity and other thermodynamic properties. Examples are given below.

Example 1 Estimate the heat capacity of carbon tetrachloride (CCl4) as a low-pressure gas at 500 K.

Substitution of the coefficients from the table and temperature into the equation for heat capacity yields: $C_P = 19.816 + 3.3311E\text{-}01*500 - 5.0511E\text{-}04*500^2 + 3.4057E\text{-}07*500^3 - 8.4249E\text{-}11*500^4$

$C_P = 97.40$ joule/(mol K)

Example 2 Calculate the energy required to heat gaseous ethyl chloride (C2H5Cl) from 300 K to 600 K at low pressure.

From thermodynamics, the change in enthalpy, ΔH, at constant pressure is:

$$\Delta H = \; C_P \, dT \; = \; (A + B*T + C*T^2 + D*T^3 + E*T^4) \, dT$$

$$\Delta H = A*T + B/2*T^2 + C/3*T^3 + D/4*T^4 + E/5*T^5 \Big]_{T_1}^{T_2}$$

Substitution of the coefficients from the table and the temperature limits into the equation provides:

$$\Delta H = 35.946*(600 - 300) + 5.2294E\text{-}02/2*(600^2 - 300^2) + 2.0321E\text{-}04/3*(600^3 - 300^3) - 2.2795E\text{-}07/4*(600^4 - 300^4) + 6.9123E\text{-}11/5*(600^5 - 300^5)$$

$\Delta H = 24{,}760$ joule/mol

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