

Chapter 4

HEAT CAPACITY OF SOLID

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ABSTRACT

Results for heat capacity of solid as a function of temperature are presented for major organic and inorganic chemicals. The results cover a wide temperature range and include many types of compounds. 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 unit operations involving solids at elevated temperatures, the heat capacity is required to determine the energy (heat) necessary to bring the solids up to the required processing temperature. Additional uses include heat exchanger and energy balance design calculations.

In this article, correlation results for heat capacity of solids 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 solid is a series expansion in temperature:

$$C_p = A + B T + C T^2 \quad (4-1)$$

where

C_p = heat capacity of solid, joule/(mol K)

A, B, C = regression coefficients for chemical compound

T = temperature, K

The results for heat capacity of solid are given in Tables 4-1 and 4-2. The tabulations are applicable to a wide variety of substances.

In preparing the compilation, a literature search was conducted to identify data source publications for organics (1-38) and inorganics (1-104). 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. For organics, many of the values are based on sources from DIPPR (4). For inorganics, many of the values are based on sources from JANAF tables (57-59) and Thermophysical Properties of Matter (23). The estimates are primarily based on empirical methods of the senior author. Experimental data and estimates were then regressed to provide the same equation for all compounds.

Very limited experimental data for solid heat capacity are available at very low temperatures. Thus, the estimated values at very low temperatures should be considered rough approximations. The values for substances that are solids at room temperature are more accurate.

A comparison of correlation and actual data values for heat capacity is shown in Figure 4-1 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 additional thermodynamic properties. Examples are given below.

Example 1 Estimate the solid heat capacity of phenol (C_6H_6O) at 298.15 K.

Substitution of the coefficients from the table and temperature into the equation for heat capacity yields:

$$C_p = 9.769 + 4.0832E-01 \cdot 298.15 - 1.9001E-05 \cdot 298.15^2$$

$$C_p = 129.82 \text{ joule/(mol K)}$$

Example 2 Calculate the energy required to heat solid naphthalene ($C_{10}H_8$) from 100 K to 300 K.

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

$$\Delta H = \int_{T_1}^{T_2} C_p dT = \int_{T_1}^{T_2} (A + B \cdot T + C \cdot T^2) dT$$

$$\Delta H = \left[A \cdot T + \frac{B}{2} \cdot T^2 + \frac{C}{3} \cdot T^3 \right]_{T_1}^{T_2}$$

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

$$\Delta H = 4.824 \cdot (300 - 100) + 5.0634 \cdot 10^{-1} \cdot (300^2 - 100^2) + 1.8503 \cdot 10^{-4} \cdot (300^3 - 100^3)$$

$$\Delta H = 22,820 \text{ joule/mol}$$

REFERENCES - ORGANIC COMPOUNDS

1-36. See **REFERENCES - ORGANIC COMPOUNDS** in **Chapter 2 HEAT CAPACITY OF GAS**

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REFERENCES - INORGANIC COMPOUNDS

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