

## Chapter 3

### HEAT CAPACITY OF LIQUID

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#### ABSTRACT

Results for heat capacity of liquid as a function of temperature are presented for major organic and inorganic chemicals. The results cover a wide temperature range and include many compound types. The agreement between correlation and data is quite good.

#### INTRODUCTION

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

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

$$C_P = A + B T + C T^2 + D T^3 \quad (3-1)$$

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

The results for heat capacity of liquid are given in Tables 3-1 and 3-2. In preparing the compilation, a literature search was conducted to identify data source publications for organics (1-43) 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 organic compounds, most of the estimates were based on group contribution (Cheuh-Swanson, 29), corresponding states (Lee-Kesler, 29) and boiling point methods (Yaws and co-workers). The relation of (heat capacity)(density)<sup>n</sup>=constant was utilized to extend both experimental data and estimates. Values of n ranged from 1/2 to 1. Experimental data and estimates were then regressed to provide the same equation for all compounds.

For inorganic compounds, many of the estimates are based on the JANAF tables (57-59), Bureau of Mines bulletins (60-63) and group contribution methods. The relation of (heat capacity)(density)<sup>n</sup>=constant was utilized to extend both experimental data and estimates.

Very limited experimental data for liquid heat capacity are available at temperatures in the region of the melting point temperature. Data in the boiling-critical point temperature interval are also very scarce. Thus, the values in the region of the melting point and in the boiling-critical point temperature interval should be considered rough approximations. The values in the intermediate region (above melting and below boiling point) are more accurate.

A comparison of correlation and actual data for liquid heat capacity is shown in Figure 3-1 for a representative chemical. The graph discloses 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 liquid heat capacity of pentane (C<sub>5</sub>H<sub>12</sub>) at 298.15 K.

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

$$C_P = 80.641 + 6.2195E-01 \cdot 298.15 - 2.2682E-03 \cdot 298.15^2 + 3.7423E-06 \cdot 298.15^3$$

$$C_P = 163.64 \text{ joule/(mol K)}$$

**Example 2** Calculate the energy required to heat liquid toluene (C<sub>7</sub>H<sub>8</sub>) from 300 K to 500 K. From

thermodynamics, the change in enthalpy,  $\Delta H$ , at constant pressure is:

$$\Delta H = C_p dT = (A + B \cdot T + C \cdot T^2 + D \cdot T^3) dT$$

$$\Delta H = A \cdot T + B/2 \cdot T^2 + C/3 \cdot T^3 + D/4 \cdot T^4 \Big|_{T_1}^{T_2}$$

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

$$\Delta H = 83.703 \cdot (500 - 300) + 5.1666 \cdot 10^{-1} / 2 \cdot (500^2 - 300^2) - 1.4910 \cdot 10^{-3} / 3 \cdot (500^3 - 300^3) + 1.9725 \cdot 10^{-6} / 4 \cdot (500^4 - 300^4)$$

$$\Delta H = 36,200 \text{ joule/mol}$$

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