

Heat capacity and enthalpy of liquids: Aromatic hydrocarbons

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THE PREPARATION OF THIS DATA ITEM

The work on this particular Data Item was monitored and guided by the Physical Data and Reaction Kinetics Committee, which first met in 1966 and now has the following membership:

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The technical work involved in the assessment of the available information and the construction and subsequent development of the Data Item was undertaken by

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The person with overall responsibility for the work in this subject area is Mr N. Thompson, Head of Fluid Mechanics and Physical Properties Group.

HEAT CAPACITY AND ENTHALPY OF LIQUIDS: AROMATIC HYDROCARBONS

1. INTRODUCTION

This Data Item presents values of saturated liquid heat capacity and enthalpy in tabular form for the aromatic hydrocarbons listed in Table I which are members of the following groups:

- (a) C_6 to C_{12} Alkylbenzenes
- (b) C_8 Alkenylbenzene
- (c) C_{12} to C_{18} Polyphenyl hydrocarbons
- (d) C_{10} to C_{14} Fused ring hydrocarbons.

The data on which these values are based are the most reliable available and the range covered is from the melting temperature to the normal boiling point or to the limit of the experimental data whichever is the higher. In common with other ESDU Data Items, quantities are expressed in SI units and conversion factors to other units are provided in Section 3.

Section 4 describes the procedure used to obtain the values of heat capacity presented and indicates the effect of pressure. Values of enthalpy have been derived from values of heat capacity as explained in Section 5. Section 6 gives an explanation of the Tables and indicates the uncertainties in the values presented in them.

Section 7 contains all the sources of data used in the preparation of this Data Item. For convenience when using these Tables, a fold-out flap attached to the last page provides an index to the Data Item, showing against the name of each compound the page and table number where the data relating to it appear.

2. NOTATION AND UNITS

The SI unit of heat capacity is the joule per kilogram kelvin (J/kg K). A convenient multiple unit for the range of heat capacities in this Data Item is the kilojoule per kilogram kelvin (kJ/kg K) and is adopted here.

a_1, a_2, a_3	constants for each liquid in Equations (4.1) and (5.1)	kJ/kg K
c	heat capacity	kJ/kg K
h	enthalpy	kJ/kg
T	thermodynamic temperature	K

Subscripts

b	denotes value at normal boiling point
c	denotes value at critical point
m	denotes value at melting point
r	denotes reduced quantity, <i>e.g.</i> $T_r = T/T_c$
s	denotes value at saturation.

3. CONVERSION FACTORS

$$\begin{aligned} 1 \text{ kJ/kg K} &= 0.239 \ 006 \text{ cal/g K} \\ &= 0.238 \ 846 \text{ Btu/lb } ^\circ\text{F} \end{aligned}$$

$$\begin{aligned} 1 \text{ kJ/kg} &= 0.239 \ 006 \text{ cal/g} \\ &= 0.429 \ 923 \text{ Btu/lb.} \end{aligned}$$

4. HEAT CAPACITY

4.1 Heat Capacity at Saturation Pressure

For many liquids it has been suggested (Reference 5) that a good representation of heat capacity data over a wide range of temperature is given by the equation

$$c_s = a_1(1 - T_r)^{-2/3} + a_2(1 - T_r)^{-1/3} + a_3. \quad (4.1)$$

For the liquids considered in this Data Item, the derived values of a_1 , a_2 and a_3 given in Table I are a correlated set of values giving the best fit to the data for the liquid aromatic hydrocarbons not only as individual compounds but also as members of their chemical series based on molecular structure and on a systematic arrangement of the isomers.

Since the available experimental data do not cover the full liquid range, the data used to evaluate the constants in Equation (4.1) have, where possible, been extended to the melting temperature and to the normal boiling point using as a guide the available data plotted on a reduced temperature scale, and the relation (Derivation 6)

$$\text{heat capacity} \times (\text{liquid density})^n = \text{constant}$$

where n is a constant for each compound.

The complete range of data for each compound was fitted by Equation (4.1) and correlations of the values of the constants with molecular structure and arrangement of the isomers were used to estimate the heat capacities of those liquids for which either very few or no data were available.

Using the values of the constants in Table I together with the values of T_c also given in Table I, values of c_s in kJ/kg K have been calculated for each compound from Equation (4.1) and are presented in Tables II to IV. Users' attention is drawn to the limits of applicability of Equation (4.1) given in Table I. Any extrapolation above the upper limit should be carried out with caution.

4.2 Effect of Pressure

The experimental data reported in each Derivation are either at 1 atm pressure or at saturation pressure. Except at temperatures very near the critical point, the differences between the values of liquid heat capacity at 1 atm pressure and at saturation pressures are not significant.

5. ENTHALPY AT SATURATION PRESSURE

Values of liquid enthalpy for each compound may be calculated from the equation,

$$h_s = -T_c \left[3a_1(1 - T_r)^{1/3} + \frac{3}{2}a_2(1 - T_r)^{2/3} + a_3(1 - T_r) \right]_{T_r^*}^{T_r} \quad (5.1)$$

obtained by integrating Equation (4.1). T_r^* denotes the reduced temperature at which the enthalpy is set to zero. The enthalpy base temperature has been taken as 25 °C = 298.15 K at which the liquid was arbitrarily assigned an enthalpy of zero. For compounds where the melting temperature is above 25 °C, Equation (5.1) has been extrapolated from the melting temperature to 25 °C in deriving the enthalpy data. The values of enthalpies in kJ/kg have been calculated for each compound from Equation (5.1) and are presented in Tables V to VII.

6. EXPLANATION OF TABLES

6.1 Notes on Compounds Considered

The compounds are numbered from 1 to 34 in the index flap of page 15 and these numbers are used to identify the compounds in the Tables where space does not permit the use of the name. The compounds are identified by a systematic name but for most compounds alternative names are given on the index flap by which the compounds may be identified in other literature.

The values of T_m , T_b and T_c for most of the compounds have been taken from Data Items 73029 and 74007. For the remaining compounds values have been taken from the literature. Compounds for which no, or few, experimental data exist and for which values of the constants were estimated as described in Section 4.1 are indicated by an asterisk against their compound number in Table I.

Tables II to IV present values of heat capacity and Tables V to VII present values of enthalpy at 10 K intervals of temperature from the melting temperature to either the normal boiling point or to the limit of the experimental data.

6.2 Accuracy of Data

The experimental data which are assessed to be the most reliable have a repeatability of about ±1 per cent, although differences in the methods used by different workers, and also in the purity of samples, can increase the uncertainties to about ±2 per cent. Reliable data are not available for all the compounds considered nor over the whole temperature range covered. The extrapolated heat capacities using liquid density data (see Section 4.1) are considered reasonably accurate up to the normal boiling point.

Although it is considered that the correlation procedures adopted keep the errors in the values presented to a minimum, the user should allow for an uncertainty of ±5 per cent in the values of heat capacity given to 3 decimal places and in the values of enthalpy given to 1 decimal place in the Tables. This uncertainty increases to ±10 per cent for the values of heat capacity given to 2 decimal places and for the values of enthalpy given to the nearest integer in the Tables.

As is to be expected since a different method of correlating the data is used here from that adopted in Data Items 73009 and 74024, there are slight differences (never exceeding 1.5 per cent in the worst case near the normal boiling point) between heat capacity values given for benzene and toluene in those Items and the values presented here.

7. REFERENCES AND DERIVATION

References

The references given are recommended sources of information supplementary to that in this Data Item.

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Derivation

The Derivation lists selected sources that have assisted in the preparation of this Data Item.

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