

Heat capacity and enthalpy of liquids: Alkanes

ESDU Copyright material. For current status contact ESDU.

Endorsed by
The Institution of Chemical Engineers
The Institution of Mechanical Engineers

 **Documents**
Document Sharing Hub

ESDU DATA ITEMS

Data Items provide validated information in engineering design and analysis for use by, or under the supervision of, professionally qualified engineers. The data are founded on an evaluation of all the relevant information, both published and unpublished, and are invariably supported by original work of ESDU staff engineers or consultants. The whole process is subject to independent review for which crucial support is provided by industrial companies, government research laboratories, universities and others from around the world through the participation of some of their leading experts on ESDU Technical Committees. This process ensures that the results of much valuable work (theoretical, experimental and operational), which may not be widely available or in a readily usable form, can be communicated concisely and accurately to the engineering community.

We are constantly striving to develop new work and review data already issued. Any comments arising out of your use of our data, or any suggestions for new topics or information that might lead to improvements, will help us to provide a better service.

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:

Chairman	
Mr C.F. Beaton	— Independent
Members	
Dr D. Ambrose*	— Independent
Dr M.W. Chase†	— National Bureau of Standards, Gaithersburgh, USA
Dr J.R. Downey†	— Dow Chemical, Midland, USA
Dr A. Gunning	— Bechtel Ltd, UK
Dr G. Hobson	— Imperial Chemical Industries Ltd, Petrochemicals & Plastics Division, Wilton, UK
Dr D.T. Jamieson	— National Engineering Laboratory, East Kilbride, UK
Mr S.R. Knight	— Stone & Webster Engineering Ltd, Milton Keynes, UK
Dr M. Schoenberg†	— Hoechst AG, Frankfurt, Germany
Dr H.J. White, Jr†	— National Bureau of Standards, Washington D.C., USA.

* Emeritus Member.

† Corresponding Member.

The technical work involved in the assessment of the available information and the construction and subsequent development of the Data Item was undertaken (under contract to ESDU) by

Mr C.F. Beaton — Independent.

The person with overall responsibility for the work in this subject area is Mr. R. Partington, Head of Internal Flow and Physical Properties Group.

HEAT CAPACITY AND ENTHALPY OF LIQUIDS: ALKANES

1. INTRODUCTION

This Data Item presents values of liquid heat capacity and enthalpy in tabular form for the straight and branched chain alkanes listed in Table I. It supersedes Item 77025 by extending the upper temperature limit to $0.96T_c$.

The data on which these values are based are the most reliable available and for most compounds the range covered is from the melting temperature to a reduced temperature of 0.96. 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 the 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.

Appendix A presents a brief discussion of the theoretical relationships between alternative definitions of heat capacity and Appendix B some typical differences between reported values at the highest valid temperature.

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	constant for each liquid in Equations (4.1) and (5.1)	kJ/kg K
a_2, a_3, a_4	non-dimensional constants for each liquid in Equations (4.1) and (5.1)	-
c	heat capacity	kJ/kg K
H	enthalpy	kJ/kg
T	thermodynamic temperature	K

Subscripts

c	denotes value at critical point
m	denotes value at melting point
p	denotes constant pressure
r	denotes reduced quantity, <i>e.g.</i> $T_r = T/T_c$.

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

It has recently been suggested (Reference 10) that heat capacity data over a range of temperature can be represented by the equation

$$c_p = a_1 [1 + a_2(1 - T_r)^{-1} + a_3(1 - T_r) + a_4(1 - T_r)^2] \quad (4.1)$$

For the liquids considered in this Data Item, the derived values of a_1 , a_2 , a_3 , and a_4 given in Table I are a correlated set of values giving the best fit to the data for the liquid alkanes not only as individual compounds but also as members of their chemical series based on molecular structure. The relationship between measured values of heat capacity and c_p is discussed in Appendix A.

Since the available experimental data do not cover the full liquid range, the data used to evaluate the constants in Equation (4.1) have been extended to the melting temperature and to the critical point using as a guide the available data plotted on a reduced temperature scale. Where necessary, values at temperatures above $0.6T_r$ have been predicted using methods recommended by Reid, Prausnitz and Sherwood, (Reference 7).

The method of Lyman and Danner, (Reference 6) was used for as many compounds as there were values of the radius of gyration. The method of Yuan and Stiel, (Reference 4) was used for the remainder. Both methods were shown to be reliable when tested against the NBS "standard" values for *n*-heptane (Derivation 43). Predicted values and the NBS values for heptane were corrected to c_p values by the methods referred to in Appendix A (Section A3). The results of San José (Derivation 67) confirmed the procedure. Data calculated by Amirkhanov *et al.* from measured values of heat capacity at constant volume for pentane, hexane, heptane and octane (Derivation 57) were also in reasonable agreement.

The first four members of the alkanes series, methane to butane, together with isobutane have been fully studied at NBS in recent years (Derivations 64, 66, 74, 75, 76) and these values were accepted as the basis of the correlation of these compounds.

The experimental data for the heat capacity of some compounds exhibit a minimum point at temperatures near the normal melting temperature; this behaviour is well established for *n*-heptane (compound no. 14), *n*-nonane (compound no. 41) and 2-methylnonane (compound no. 49). The four-constant equation could not reproduce this effect while accurately representing data at higher temperatures. An appropriate start temperature is given in these cases and values at lower temperatures are preceded by the letter x.

The range of available experimental data for each compound is indicated in the following tables by values given to three decimal places. Predicted values are given to two decimal places.

Using the values of the constants in Table I together with the values of T_c also given in Table I, values of c_p , in kJ/kg K have been calculated for each compound from Equation (4.1) and are presented in Table II. User's attention is drawn to the limits of validity of Equation (4.1) given in Table I. Any extrapolation to

higher temperatures beyond those limits should be carried out with caution as such an extrapolation may give high values of c_p for some compounds.

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 exceeding $0.9 T_c$, the differences between the values of liquid heat capacity at 1 atm pressure and at saturation pressure are not significant.

5. ENTHALPY AT SATURATION PRESSURE

Although it is not thermodynamically correct, values of liquid enthalpy for each compound may be calculated from the equation,

$$H_s = -a_1 T_c \left[(1 - T_r) + a_2 \log_e (1 - T_r) + \frac{1}{2} a_3 (1 - T_r)^2 + \frac{1}{3} a_4 (1 - T_r)^3 \right] \frac{T_r}{T_r^*} \quad (5.1)$$

obtained by integrating Equation (4.1). T_r^* denotes the reduced temperature at which the enthalpy is set to zero. The values obtained were within the accuracy claimed up to a reduced temperature of 0.96. The enthalpy base temperature for methane and ethane has been taken as the melting temperature and for all other compounds has been taken as 298.15 K at which the liquid was arbitrarily assigned an enthalpy of zero. For compounds where the melting temperature is above 298.15 K, Equation (5.1) has been extrapolated from the melting temperature to 298.15 K 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 Table III.

6. EXPLANATION OF TABLES

6.1 Notes on Compounds Considered

The compounds are numbered from 1 to 70 in Table I and these numbers are used to identify the compounds in the subsequent 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 by which the compounds may be identified in other literature. The names in bold type are those based on BSI recommendations, see References 3 and 5.

The values of T_m and T_c for most compounds have been taken from Data Items 84022, 84028 and 85002. For the others, the values have been taken from other literature or estimated. Compounds for which no, or few, experimental data exist and for which values of the constants for Equation (4.1) were estimated as described in Section 4.1 are indicated by an asterisk against their compound number in Table I.

Table II presents values of heat capacity and Table III presents values of enthalpy at 10 K intervals of temperature and the range covered is from the melting temperature or an appropriate starting temperature to a reduced temperature of 0.96.

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 method used by different workers, and also in the purity of the samples can

increase the uncertainties to ± 2 per cent. Reliable data are not available for all the compounds considered nor over the whole temperature range covered. The prediction procedures are within ± 3 per cent of experimental data (where available) but could be considerably less accurate at temperatures in excess of $T_r = 0.9$.

In Appendix A, thermodynamic definitions of three values of heat capacity are given but only one of these is normally measured. However the differences between the numerical values of heat capacity from all three definitions are insignificant below a reduced temperature of 0.8. Hence experimental data measured below this temperature are valid and were used for the correlation. The values of enthalpy obtained by integrating Equation (4.1) were checked against values reported by workers using an equation of state (Reference 8 and Derivations 64, 66, 68, 71–77 and 80). An indication of the differences between the results reported here and those found in the literature at the highest valid temperature is given in Appendix B.

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 ± 3 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 ± 5 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.

7. REFERENCES AND DERIVATION

References

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

1. TIMMERMANS, J. *Physico-chemical constants of pure organic compounds*. Vol. 1, Elsevier, New York, 1950.
2. TIMMERMANS, J. *Physico-chemical constants of pure organic compounds*. Vol. 2, Elsevier, New York, 1965.
3. BSI *Recommended names for chemicals in industry*. British Standards Institution, BS2474: 1965.
4. YUAN, T.
STIEL, L.I. Heat capacity of saturated nonpolar and polar liquids. *Ind. Eng. Chem. Fundam.*, Vol. 9, No. 3, pp. 393–400, 1970.
5. HMSO *Classification of chemicals in the Brussels nomenclature and in the United Kingdom customs and excise tariff*. HMSO, London, UK, 1973.
6. LYMAN, T.J.
DANNER, R.P. Correlation of liquid heat capacities with a four-parameter corresponding states method. *AIChEJ.*, Vol. 22, No. 4, pp. 759–765, 1976.
7. REID, R.C.
PRAUSNITZ, J.M.
SHERWOOD, T.K. *The properties of gases and liquids*. 3rd Edition, McGraw-Hill, New York, 1977.
8. REYNOLDS, W.C. *Thermodynamic properties in S.I.* Stanford University, California, USA, 1979.
9. ROWLINSON, J.S.
SWINTON, F.L. *Liquids and liquid mixtures*. Butterworths Scientific, London, 1981.
10. WATSON, J.T.R. Private communication. National Engineering Laboratory, East Kilbride, UK, 1985.

Derivation

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

11. WIEBE, R.
HUBBARD, K.H.
BREVOORT, M.J. The heat capacity of saturated liquid ethane from the boiling point to the critical temperature and heat of fusion of the solid. *J. Am. Chem. Soc.*, Vol. 52, No. 2, pp. 611–622, 1930.
12. WIEBE, R.
BREVOORT, M.J. The heat capacity of saturated liquid nitrogen and methane from the boiling point to the critical temperature. *J. Am. Chem. Soc.*, Vol. 52, No. 2, pp. 622–633, 1930.
13. PARKS, G.S.
HUFFMAN, H.M.
THOMAS, S.B. Thermal data on organic compounds. VI. The heat capacities, entropies and free energies of some saturated non-benzenoid hydrocarbons. *J. Am. Chem. Soc.*, Vol. 52, No. 3, pp. 1032–1041, 1930.
14. HUFFMAN, H.M.
PARKS, G.S.
THOMAS, S.B. Thermal data on organic compounds. VIII. The heat capacities, entropies and free energies of the isomeric heptanes. *J. Am. Chem. Soc.*, Vol. 52, No. 8, pp. 3241–3251, 1930.
15. HUFFMAN, H.M.
PARKS, G.S.
BARMORE, M. Thermal data on organic compounds. X. Further studies on the heat capacities, entropies and free energies of hydrocarbons. *J. Am. Chem. Soc.*, Vol. 53, No. 10, pp. 3876–3888, 1931.
16. SPAGHT, M.E.
THOMAS, S.B.
PARKS, G.S. Some heat-capacity data on organic compounds obtained with a radiation calorimeter. *J. Phys. Chem.*, Vol. 36, No. 3, pp. 882–888, 1932.
17. RICHARDS, W.T.
WALLACE, J.H. The specific heats of five organic liquids from their adiabatic temperature – pressure coefficients. *J. Am. Chem. Soc.*, Vol. 54, No. 7, pp. 2705–2713, 1932.
18. PARKS, G.S.
LIGHT, D.W. Thermal data on organic compounds. XIII. The heat capacities and entropies of *n*-tetradecane and the hydroxybenzoic acids. The relative free energies of some benzenoid position isomers. *J. Am. Chem. Soc.*, Vol. 56, No. 7, pp. 1511–1513, 1934.
19. ASTON, J.G.
MESSERLY, G.H. Heat capacities and entropies of organic compounds. II. Thermal and vapor pressure data for tetramethylmethane from 13.22 K to the boiling point. The entropy from its Raman spectrum. *J. Am. Chem. Soc.*, Vol. 58, No. 12, pp. 2354–2361, 1936.
20. WITT, R.K.
KEMP, J.D. The heat capacity of ethane from 15 K to the boiling point. The heat of fusion and the heat of vaporization. *J. Am. Chem. Soc.*, Vol. 59, No. 2, pp. 273–276, 1937.
21. PARKS, G.S.
SHOMATE, C.H.
KENNEDY, W.D.
CRAWFORD, B.I. The entropies of *n*-butane and isobutane with some heat capacity data for isobutane. *J. Chem. Phys.*, Vol. 5, No. 5, pp. 359–363, 1937.

22. KEMP, J.D.
EGAN, C.J. Hindered rotation of the methyl groups in propane. The heat capacity, vapor pressure, heats of fusion and vaporization of propane. Entropy and density of the gas. *J. Am. Chem. Soc.*, Vol. 60, No. 7, pp. 1521–1525, 1938.
23. PITZER, K.S. The thermodynamics of *n*-heptane and 2,2,4-trimethylpentane, including heat capacities, heats of fusion and vaporization and entropies. *J. Am. Chem. Soc.*, Vol. 62, No. 5, pp. 1224–1227, 1940.
24. ASTON, J.G.
MESSERLY, G.H. The heat capacity and entropy, heats of fusion and vaporization and the vapor pressure of *n*-butane. *J. Am. Chem. Soc.*, Vol. 62, No. 8, pp. 1917–1923, 1940.
25. ASTON, J.G.
KENNEDY, R.M.
SCHUMANN, S.C. The heat capacity and entropy, heats of fusion and vaporization and the vapor pressure of isobutane. *J. Am. Chem. Soc.*, Vol. 62, No. 8, pp. 2059–2063, 1940.
26. MESSERLY, G.H.
KENNEDY, R.M. The heat capacity and entropy, heats of fusion and vaporization and the vapor pressure of *n*-pentane. *J. Am. Chem. Soc.*, Vol. 62, No. 11, pp. 2988–2991, 1940.
27. PARKS, G.S.
WEST, T.J.
MOORE, G.E. Thermal data on organic compounds. XXI. Some heat capacity, entropy and free energy data for the four methylnonanes. *J. Am. Chem. Soc.*, Vol. 63, No. 4, pp. 1133–1135, 1941.
28. PITZER, K.S.
SCOTT, D.W. The thermodynamics of branched-chain paraffins. The heat capacity, heat of fusion and vaporization, and entropy of 2,3,4-trimethylpentane. *J. Am. Chem. Soc.*, Vol. 63, No. 9, pp. 2419–2422, 1941.
29. SCHUMANN, S.C. The heat capacity and entropy, heats of fusion and vaporization and the vapor pressure of isopentane. University Microfilms Pub. 241, pp. 1–84, 1941.
30. KENNEDY, R.M. The heat capacity and entropy, heats of vaporization and the vapor pressure of isobutane, tetramethyl and dimethyl ether. Hindered rotation and molecular structure. University Microfilms Pub. 353, No. 5, pp. 1–86, 1941.
31. SCHUMANN, S.C.
ASTON, J.G.
SAGENKAHN, M. The heat capacity and entropy, heats of fusion and vaporization and the vapor pressures of isopentane. *J. Am. Chem. Soc.*, Vol. 64, No. 5, pp. 1039–1043, 1942.
32. GUTHRIE, G.B.
HUFFMAN, H.M. Thermal data. XVI. The heat capacity and entropy of isopentane. The absence of a reported anomaly. *J. Am. Chem. Soc.*, Vol. 65, No. 6, pp. 1139–1143, 1943.
33. KILPATRICK, J.E.
PITZER, K.S. The thermodynamics of 2,2-dimethylbutane, including the heat capacity, heats of transitions, fusion and vaporization and the entropy. *J. Am. Chem. Soc.*, Vol. 68, No. 6, pp. 1066–1072, 1946.
34. DOUSLIN, D.R.
HUFFMAN, H.M. Low-temperature thermal data on the five isomeric hexanes. *J. Am. Chem. Soc.*, Vol. 68, No. 9, pp. 1704–1708, 1946.

35. OSBORNE, N.S.
GINNINGS, D.C. Measurements of heat of vaporization and the heat capacity of a number of hydrocarbons. *J. Res. Nat. Bur. Stand.*, Vol. 39, No. 5, pp. 453–477, 1947.
36. PARKS, G.S.
MOORE, G.E.
RENQUIST, M.L.
NAYLOR, B.F.
McCLAIN, L.A.
FUJII, P.S.
HATTON, J.A. Thermal data on organic compounds. XXV. Some heat capacity, entropy and free energy data for nine hydrocarbons of high molecular weight. *J. Am. Chem. Soc.*, Vol. 71, No. 10, pp. 3386–3389, 1949.
37. AUERBACH, C.E.
SAGE, B.H.
LACEY, W.N. Isobaric heat capacities at bubble point. Propene, neohexane, cyclohexane and iso-octane. *Ind. Eng. Chem.*, Vol. 42, No. 1, pp. 110–113, 1950.
38. CONNOLLY, T.J.
SAGE, B.H.
LACEY, W.N. Isobaric heat capacities at bubble point. *n*-Hexane, methylcyclopentane and *n*-octane. *Ind. Eng. Chem.*, Vol. 43, No. 4, pp. 946–950, 1951.
39. SCOTT, D.W.
DOUSLIN, D.R.
GROSS, M.E.
OLIVER, G.D.
HUFFMAN, H.M. 2,2,3,3-Tetramethylbutane: Heat capacity, heats of transition, fusion and sublimation, vapor pressure, entropy and thermodynamic functions. *J. Am. Chem. Soc.*, Vol. 74, No. 4, pp. 883–887, 1952.
40. SCHLINGER, W.G.
SAGE, B.H. Isobaric heat capacities at bubble point. *cis*-2-Butene, isopropylbenzene and *n*-decane. *Ind. Eng. Chem.*, Vol. 44, No. 10, pp. 2454–2456, 1952.
41. GINNINGS, D.C.
FURUKAWA, G.T. Heat capacity standards for the range 14 to 1200 K. *J. Am. Chem. Soc.*, Vol. 75, No. 3, pp. 522–527, 1953.
42. FINKE, H.L.
GROSS, M.E.
WADDINGTON, G.
HUFFMAN, H.M. Low-temperature thermal data for the nine normal paraffin hydrocarbons from octane to hexadecane. *J. Am. Chem. Soc.*, Vol. 76, No. 2, pp. 333–341, 1954.
43. DOUGLAS, T.B.
FURUKAWA, G.T.
McCOSKEY, R.E.
BALL, A.F. Calorimetric properties of normal heptane from 0 to 520 K. *J. Res. Nat. Bur. Stand.*, Vol. 53, No. 3, pp. 139–153, 1954.
44. STAVELEY, L.A.K.
WARREN, J.B.
PAGET, H.P.
DOWRICK, D.J. Some thermodynamic properties of compounds of the formula MX_4 . Part II. Tetra-alkyl compounds. *J. Chem. Soc.*, pp. 1992–2001, 1954.
45. HELFREY, P.F.
HEISER, D.A.
SAGE, B.H. Isobaric heat capacities at bubble point. Two trimethylbenzenes and *n*-heptane. *Ind. Eng. Chem.*, Vol. 47, No. 11, pp. 2385–2388, 1955.

46. HESTERMANS, P.
WHITE, D. The vapor pressure, heat of vaporization and heat capacity of methane from the boiling point to the critical temperature. *J. Phys. Chem.*, Vol. 65, No. 2, pp. 362–365, 1961.
47. HUFFMAN, H.M.
GROSS, M.E.
SCOTT, D.W.
McCULLOUGH, J.P. Low temperature thermodynamic properties of six isomeric heptanes. *J. Phys. Chem.*, Vol. 65, No. 3, pp. 495–503, 1961.
48. McCULLOUGH, J.P.
MESSERLY, J.F. The chemical thermodynamic properties of hydrocarbons and related substances. *US Bur. Mines Bull.*, No. 596, pp. 1–15, 1961.
49. MESSERLY, J.F.
GUTHRIE, G.B.
TODD, S.S.
FINKE, H.L. Low-temperature thermal data for pentane, *n*-heptadecane, and *n*-octadecane. Revised thermodynamic functions for the *n*-alkanes C₅–C₁₈. *J. Chem. Eng. Data*, Vol. 12, No. 3, pp. 338–346, 1967.
50. ZOTOV, V.V.
NERUCHEV, Yu, A
OTPUSHCENNIKOV, N.F. Some thermodynamic properties of *n*-heptane on the saturation line. (In Russian). *Inzh. Fiz. Zh.*, Vol. 15, No. 5, pp. 890–892, 1968. (Eng. Trans, pp. 1098–1099).
51. SUGISAKI, M.
ADACHI, K.
SUGA, H.
SEKI, S. On the glass transition phenomenon of isopentane. *Bull. Chem. Soc. Japan*, Vol. 41, No. 3, pp. 593–600, 1968.
52. RECKO, W.M. Adiabatic calorimeter for measurement of the specific heat capacity of liquids. (In Russian). *Bull. Acad. Pol. Sci., Ser. Sci. Chim.*, Vol. 16, No. 10, pp. 543–548, 1968.
53. ENOKIDO, H.
SHINODA, T.
MASHIKO, Y.-I. Thermodynamic properties of neopentane from 4 K to the melting point and comparison with spectroscopic data. *Bull. Chem. Soc. Japan*, Vol. 42, No. 1, pp. 84–91, 1969.
54. MUSTAFAEV, R.A. Temperature dependence of some thermophysical values of liquid *n*-alkanes at atmospheric pressure. (In Russian). *Izv. Vyssh. Ucheb. Zaved., Neft. Gaz.*, Vol. 11, No. 6, pp. 75–78, 1968.
55. YESAVAGE, V.F.
KATZ, D.L.
POWERS, J.E. Thermal properties of propane. *J. Chem. Eng. Data*, Vol. 14, No. 2, pp. 197–204, 1969.
56. TOULOUKIAN, Y.S.
MAKITA, T. *Thermophysical properties of matter*. The TPRC Data Series, Vol. 6 – Specific heat of non-metallic liquids and gases. IFI/Plenum, New York, 1970 and 1976 (Supplement).
57. AMIRKHANOV, Kh.I.
ALIBEKOV, B.G.
VIKHROV, D.I.
MIRSKAYA, V.A.
LEVINA, L.N. Isobaric heat capacity of *n*-pentane, *n*-hexane, *n*-heptane, and *n*-octane along the boundary curve of the liquid. (In Russian). *Teplofiz. Vys. Temp.*, Vol. 9, No. 6, pp. 1310–1313, 1971. (Eng. Trans. pp. 1211–1214).

58. MESSERLY, J.F.
FINKE, H.L. Low-temperature thermal properties of 2-methylheptane and 2-methyldecane: The thermodynamic properties of the 2-methyl alkanes. *J. Chem. Thermodyn.*, Vol. 3, No. 5, pp. 675–687, 1971.
59. ADACHI, K.
SUGA, H.
SEKI, S. Calorimetric study of the glassy state. VI. Phase changes in crystalline and glassy-crystalline 2,3-dimethylbutane. *Bull. Chem. Soc. Japan*, Vol. 44, No. 1, pp. 78–89, 1971.
60. VAN MILTENBURG, J.C. Construction of an adiabatic calorimeter. Thermodynamic properties of standard *n*-heptane from 155 to 270 K and of 2,2-dichloropropane from 135 to 270 K. *J. Chem. Thermodyn.*, Vol. 4, No. 5, pp. 773–782, 1972.
61. FINKE, H.L.
MESSERLY, J.F. 3-Methylpentane and 3-methylheptane: Low-temperature thermodynamic properties. *J. Chem. Thermodyn.*, Vol. 5, No. 2, pp. 247–257, 1973.
62. YOUNGLOVE, B.A. The specific heats, C_p , and C_v , of compressed and liquefied methane. *J. Res. Nat. Bur. Stand. A*, Vol. 78, No. 3, pp. 401–410, 1974.
63. PETIT, J.C.
TER MINASSIAN, L. Measurements of $(\partial V/\partial T)_p$, $(\partial V/\partial p)_T$, and $(\partial H/\partial T)_p$ by flux calorimetry. *J. Chem. Thermodyn.*, Vol. 6, No. 12, pp. 1139–1152, 1974.
64. GOODWIN, R.D. Thermophysical properties of methane from 90 to 500 K at pressures to 700 bar. National Bureau of Standards Technical Note 653, National Bureau of Standards, Washington D.C., USA, 274 pp., 1974.
65. GRIGOR'EV, B.A.
RASTORGUEV, Yu.L.
YANIN, G.S. Experimental investigations of the isobaric heat capacity of *n*-alkanes. (In Russian). *Izv. Vyssh. Ucheb. Zaved., Neft. Gaz.*, Vol. 18, No. 10, pp. 63–66, 1975.
66. GOODWIN, R.D.
RODER, H.M.
et al. Thermophysical properties of ethane from 90 to 600 K at pressures to 700 bar. National Bureau of Standards Technical Note 684, National Bureau of Standards, Washington D.C., USA, 319 pp., 1976.
67. SAN JOSE, J.L.
MELLINGER, G.
REID, R.C. Measurement of the isobaric heat capacity of liquids and certain mixtures above the normal boiling point. *J. Chem. Eng. Data*, Vol. 21, No. 4, pp. 414–417, 1976.
68. ANGUS, S.
ARMSTRONG, B.
de REUCK, K.M. *International thermodynamic tables of the fluid state – methane*, No. 5: Chemical Data Series No. 16, Pergamon Press, Oxford, 251 pp., 1976.
69. FINKE, H.L.
MESSERLY, J.F.
DOUSLIN, D.R. Low-temperature thermal quantities for five alkyl – substituted pentanes. *J. Chem. Thermodyn.*, Vol. 8, No. 10, pp. 965–983, 1976.
70. ANDON, R.J.L.
MARTIN, J.F. Thermodynamic properties of hexacosane. *J. Chem. Thermodyn.*, Vol. 8, No. 12, pp. 1159–1166, 1976.

71. DAS, T.R.
REED, C.O.
EUBANK, P.T. *PVT surface and thermodynamic properties of n-pentane. J. Chem. Eng. Data*, Vol. 22, No. 1, pp. 3–9, 1977.
72. DAS, T.R.
REED, C.O.
EUBANK, P.T. *PVT surface and thermodynamic properties of isopentane. J. Chem. Eng. Data*, Vol. 22, No. 1 pp. 9–15, 1977.
73. DAS, T.R.
REED, C.O.
EUBANK, P.T. *PVT surface and thermodynamic properties of neopentane, J. Chem. Eng. Data*, Vol. 22, No. 1, pp. 16–21, 1977.
74. GOODWIN, R.D.
HAYNES, W.M. Thermophysical properties of propane from 85 to 700 K at pressures to 70 MPa. National Bureau of Standards Monograph 170, National Bureau of Standards, Washington D.C., USA, 249 pp., 1982.
75. HAYNES, W.M.
GOODWIN, R.D. Thermophysical properties of butane from 135 to 700 K at pressures to 70 MPa. National Bureau of Standards Monograph 169, National Bureau of Standards, Washington D.C., USA, 197 pp., 1982.
76. HAYNES, W.M.
GOODWIN, R.D. Thermophysical properties of isobutane from 114 to 700 K at pressures to 70 MPa. National Bureau of Standards Technical Note 1051, National Bureau of Standards, Washington D.C., USA. 196 pp., 1982.
77. GRIGOR'EV, B.A.
GERASIMOV, A.A.
KURUKOV, D.S.
VASIL'EV, Yu.-P. Study of the thermodynamic properties of hexane along the saturation line (In Russian). *Ul'trazvuk. Termodinam. Svoistva Veshch. Kursk Gos. Pedagog. Inst., Kursk*, pp. 22–29, 1983.
78. GRIGOR'EV, B.A.
ANDOLENKO, R.A. Investigation of the isobaric heat capacity of n-paraffin hydrocarbons at atmospheric pressure. (In Russian). *Izv. Vyssh. Ucheb. Zaved., Neft. Gaz.*, Vol. 27, No. 2, pp. 60–62, 1984.
79. TRC TRC Thermodynamic Tables - Hydrocarbons. Thermodynamics Research Center, Texas A & M University System, College Station, TX/National Institute of Standards and Technology, Boulder, CO, Extant 2000.
80. VAS'KOV, E.T. Thermodynamic properties of n-butane. (In Russian). *Inzh. Fiz. Zh.*, Vol. 47, No. 3, pp. 407–410, 1984.



86007

THIS PAGE IS
INTENTIONALLY
BLANK

ESDU Copyright material. For current status contact ESDU.

TABLE I (Part 1)

LIST of COMPOUNDS

The Empirical Formula, Name, Alternative Name, if any, and location of the Tables giving the Liquid Heat Capacity at Constant Pressure, c_p , and the Liquid Enthalpy at Saturation Pressure, H_s , for each compound considered in this Data Item are as follows. An asterisk against the compound name indicates that there are no experimental data for that compound.

No. Emp. Form.	Name	Alternative Name	Table Pages c_p H_s
C ₁ TO C ₃ ALKANES			
1	CH ₄ Methane		16 29
2	C ₂ H ₆ Ethane		16 29
3	C ₃ H ₈ Propane		16 29
C ₄ ALKANES			
4	C ₄ H ₁₀ Butane	n-Butane	17 30
5	2-Methylpropane	Isobutane	17 30
C ₅ ALKANES			
6	C ₅ H ₁₂ Pentane	n-Pentane	17 30
7	2-Methylbutane	Isopentane	17 30
8	2,2-Dimethylpropane	Neopentane	17 30
C ₆ ALKANES			
9	C ₆ H ₁₄ Hexane	n-Hexane	18 31
10	2-Methylpentane	Isohexane	18 31
11	3-Methylpentane		18 31
12	2,2-Dimethylbutane	Neohexane	18 31
13	2,3-Dimethylbutane	Diisopropyl	18 31
C ₇ ALKANES			
14	C ₇ H ₁₆ Heptane	n-Heptane	19 32
15	2-Methylhexane		19 32
16	3-Methylhexane		19 32
17	3-Ethylpentane	Triethylmethane	19 32
18	2,2-Dimethylpentane		20 33
19	2,3-Dimethylpentane		20 33
20	2,4-Dimethylpentane		20 33
21	3,3-Dimethylpentane		20 33
22	2,2,3-Trimethylbutane		20 33
C ₈ ALKANES			
23	C ₈ H ₁₈ Octane	n-Octane	21 34
24	2-Methylheptane		21 34
25	3-Methylheptane		21 34
26	4-Methylheptane		21 34
27	*3-Ethylhexane		21 34
28	*2,2-Dimethylhexane		22 35
29	*2,3-Dimethylhexane		22 35
30	*2,4-Dimethylhexane		22 35
31	2,5-Dimethylhexane		22 35
32	3,3-Dimethylhexane		22 35
33	*3,4-Dimethylhexane		22 35
34	*2-Methyl-3-ethylpentane		23 36
35	*3-Methyl-3-ethylpentane		23 36
36	*2,2,3-Trimethylpentane		23 36
37	2,2,4-Trimethylpentane	Isooctane	23 36
38	2,3,3-Trimethylpentane		23 36
39	2,3,4-Trimethylpentane		23 36
40	2,2,3,3-Tetramethylbutane		23 36

TABLE I (Part 2)

CONSTANTS in EQUATIONS (1) and (2)

This Table lists the constants for each compound that, when used in Equations (1) and (2), within the range of validity indicated, give the Liquid Heat Capacity at Constant Pressure, c_p , and the Liquid Enthalpy at Saturation Pressure, H_g , respectively. An asterisk against the compound name indicates that the constants a_1 , a_2 , a_3 , and a_4 are estimated, see Section 4.

No.	Name	T_c K	a_1	a_2	a_3	a_4	Range of Validity K
C₁ TO C₃ ALKANES							
1	Methane	190.56	2.9399	0.0812	0.115	-0.349	91 to 180
2	Ethane	305.33	2.4604	0.0550	-0.540	0.447	90 to 290
3	Propane	369.85	2.6353	0.0352	-0.850	0.571	85 to 350
C₄ ALKANES							
4	Butane	425.25	2.9773	0.0190	-1.015	0.690	180 to 410
5	2-Methylpropane	407.85	2.4983	0.0310	-0.500	-0.030	113 to 390
C₅ ALKANES							
6	Pentane	469.80	3.1900	0.0130	-1.115	0.744	143 to 450
7	2-Methylbutane	460.45	3.0916	0.0130	-1.040	0.570	113 to 440
8	2,2-Dimethylpropane	433.75	2.9898	0.0130	-1.040	0.547	257 to 410
C₆ ALKANES							
9	Hexane	507.90	3.3568	0.0095	-1.143	0.740	178 to 480
10	2-Methylpentane	497.85	3.2772	0.0095	-1.090	0.580	119 to 470
11	3-Methylpentane	504.45	3.2722	0.0095	-1.090	0.580	120 to 480
12	2,2-Dimethylbutane	489.35	3.1845	0.0095	-1.090	0.565	173 to 470
13	2,3-Dimethylbutane	500.25	3.2272	0.0095	-1.090	0.565	144 to 470
C₇ ALKANES							
14	Heptane	540.15	3.4542	0.0075	-1.142	0.720	210 to 520
15	2-Methylhexane	530.35	3.4005	0.0075	-1.090	0.560	155 to 500
16	3-Methylhexane	535.25	3.4266	0.0075	-1.090	0.560	160 to 510
17	3-Ethylpentane	540.65	3.3943	0.0075	-1.090	0.553	154 to 510
18	2,2-Dimethylpentane	520.55	3.3665	0.0075	-1.090	0.514	149 to 490
19	2,3-Dimethylpentane	537.35	3.3802	0.0075	-1.090	0.530	130 to 510
20	2,4-Dimethylpentane	519.75	3.4099	0.0075	-1.090	0.514	154 to 490
21	3,3-Dimethylpentane	536.35	3.3723	0.0075	-1.090	0.514	139 to 510
22	2,2,3-Trimethylbutane	531.15	3.3003	0.0075	-1.090	0.530	248 to 500
C₈ ALKANES							
23	Octane	568.95	3.5239	0.0063	-1.124	0.669	216 to 540
24	2-Methylheptane	559.65	3.4847	0.0063	-1.070	0.540	164 to 530
25	3-Methylheptane	563.65	3.4736	0.0063	-1.070	0.540	153 to 540
26	4-Methylheptane	561.75	3.4762	0.0063	-1.070	0.540	152 to 530
27	*3-Ethylhexane	565.45	3.4279	0.0063	-1.070	0.520	160 to 530
28	*2,2-Dimethylhexane	549.85	3.4454	0.0063	-1.070	0.477	152 to 520
29	*2,3-Dimethylhexane	563.45	3.4749	0.0063	-1.070	0.495	160 to 530
30	*2,4-Dimethylhexane	553.55	3.5086	0.0063	-1.070	0.477	160 to 530
31	2,5-Dimethylhexane	550.05	3.4725	0.0063	-1.070	0.495	182 to 520
32	3,3-Dimethylhexane	562.05	3.4843	0.0063	-1.070	0.495	147 to 530
33	*3,4-Dimethylhexane	568.85	3.4980	0.0063	-1.070	0.495	150 to 530
34	*2-Methyl-3-ethylpentane	567.05	3.5674	0.0063	-1.070	0.470	158 to 530
35	*3-Methyl-3-ethylpentane	576.55	3.5221	0.0063	-1.070	0.470	182 to 530
36	*2,2,3-Trimethylpentane	563.55	3.4035	0.0063	-1.070	0.495	161 to 530
37	2,2,4-Trimethylpentane	543.85	3.3577	0.0063	-1.070	0.446	166 to 520
38	2,3,3-Trimethylpentane	573.55	3.4624	0.0063	-1.070	0.524	172 to 540
39	2,3,4-Trimethylpentane	566.45	3.4950	0.0063	-1.070	0.465	164 to 540
40	2,2,3,3-Tetramethylbutane	568.15	3.3769	0.0063	-1.070	0.590	374 to 540