SPECIFIC HEAT AND ENTHALPY OF SATURATED HYDROCARBONS (ALKANES) IN THE IDEAL GAS STATE

N. M. Kuznetsov[1] and S. M. Frolov[1,2]

[1]N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation
[2]Scientific Research Institute for System Analysis, Russian Academy of Sciences, 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation

Abstract: Analytical dependences of the specific heat and enthalpy of saturated hydrocarbons in the ideal gas state on temperature and on the number of carbon atoms in a molecule up to $n = 20$ are proposed. The dependences are based on an analysis of the structure of chemical bonds in saturated hydrocarbon molecules. Thus, an increase in the number n by one at the initial value $n \geq 2$ corresponds to the addition of one CH_2 radical to the molecule. For $n \geq 4$, only CH_2 radicals can be the nearest neighbors of the added radical since edge CH_3 radicals already have such neighbors. In this case, in structural terms, the $C_{n+1}H_{2n+4}$ molecule differs from the C_nH_{2n+2} molecule in that the number of CH_2 radicals not adjacent to the edge radicals is one more. Therefore, when neglecting interaction with farther neighbors, the addition of the CH_2 radical for $n \geq 4$ leads to a linear dependence of the specific heat and enthalpy on the number n on isotherms. Excellent agreement is obtained with tabulated reference data: the error in calculating the specific heat and enthalpy in the range of 298.16–1500 K for alkanes above n-butane is comparable to the error of four-digit reference data and does not exceed 0.1%.

Keywords: alkanes; specific heat; enthalpy; ideal gas; analytical dependence; approximation error

DOI: 10.30826/CE20130212

Table Captions

Table 1 The approximation accuracy of Eqs. (4) and (5) for the ideal gas specific heats of n-pentane and n-hexane

Table 2 The approximation accuracy of Eqs. (3), (6) for the ideal gas specific heat of n-butane, n-heptane, and n-decane

Table 3 The approximation accuracy of Eqs. (3), (6) for the ideal gas specific heat of n-pentadecane and eicosan

Table 4 The approximation accuracy of Eqs. (3), (6) for the ideal gas specific heat of propane

Table 5 The approximation accuracy of Eq. (10) for calculating the ideal gas enthalpy for $n = 4$–7, 10, 15, and 20 at $T_1 = 300$ K

Table 6 The approximation accuracy of Eq. (11) for calculating the ideal gas enthalpy for $n = 4$, 7, and 10 at different temperatures

Table 7 The approximation accuracy of Eq. (11) for calculating the ideal gas enthalpy for $n = 15$ and 20 at different temperatures

Acknowledgments

The work was supported by the subsidy given to the N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences to implement the state assignment on the topic No. 0082-2016-0011 “Fundamental studies of conversion processes of energetic materials and development of scientific grounds of controlling these processes” (Registration No. AAAA-A17-117040610346-5) and to the Scientific Research Institute for System Analysis of the Russian Academy of Sciences to implement the state assignment on the topic No. 0065-2019-0005 “Mathematical modeling of dynamic processes in deformed and reactive media using multiprocessor computational systems” (Registration No. AAAA-A19-119011590092-6), and partly by the Russian Foundation for Basic Research (project 18-08-00076a).

References

1. Vargaftik, N. B. 1963. *Spravochnik po teplofizicheskim svoystvam gazov i zhidkostey* [Textbook on thermophysical properties of gases and liquids]. 1st ed. Moscow: Gosudarstvennoe izdatel'stvo fiziko-matematicheskoy literatury. 708 p.

Received March 12, 2020

Contributors

Kuznetsov Nikolay M. (b. 1929) — Doctor of Science in physics and mathematics, professor, chief research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; N-M-Kuznetsov@yandex.ru

Frolov Sergey M. (b. 1959) — Doctor of Science in physics and mathematics, head of department, head of laboratory, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; senior research scientist, Scientific Research Institute for System Analysis, Russian Academy of Sciences, 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; smfrol@chph.ras.ru