THE ENERGY OF INTERMOLECULAR FORCES IN LIQUID HALOALKANES AND THEIR BINARY MIXTURES

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Measurements of the sound speed (0.1%), the density (0.05%), and the isobaric heat capacity (2%) of liquid halogenated alkanes and their binary mixtures were evaluated in the temperature range (25-150) ^{o}C and used to calculate the energy of intermolecular forces in these liquid haloalkanes and their binary mixtures.It is shown that in these compounds in addition to the dispersion forces of attraction ($m = 6$) and repulsive forces ($n = 12$) manifest themselves the long-range bonding forces causing a dimer association of particles. The energy of the intermolecular forces is determined by the relation:

$$|E_p| = B\rho^2 + b\rho^{1/3}\left(1 - \left(\frac{\rho}{\rho_b}\right)^{11/3}\right),$$

where B and b are the dispersion and bounding force constants (determined by critical parameters), ρ is the density of a liquid, and ρ_b is the density at the normal boiling point. The expression in brackets takes into account the contribution of the energy of the repulsive forces.

On the base of the atom-atom interaction mechanism, a formula was obtained for predicting the value of the dispersion-force constant from the data on the individual properties of the atomic centers:

$$B = B_0\left(\frac{(1-\chi)\,\mu_l + \frac{l+1}{n+1}\chi\mu_n}{\mu_l}\right)^3 \left(\xi^2 + (1-\xi)^2\, a + 2\xi\,(1-\xi)\,\sqrt{a}\right).$$

Here n – is the number of the n-alkane, l – is the number of n-alkyl present in the mixture, χ – the weight concentration of n-alkyl, ξ – is the value characterizing the concentration of hydrogen atoms in the mixture.

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1. Korotkovskii V.I. , Ryshkova O.S. , Neruchev Yu.A. , Goncharov A.L., Postnikov E.B. Isobaric Heat Capacity, Isothermal Compressibility and Fluctuational Properties of 1-Bromoalkanes // Int .J. Thermophys. 2016. V. 37:58.
2. Ryshkova O.S. , Bolotnikov M.F., Korotkovskiy V.I. , Neruchev Yu.A. Peculiarities of temperature dependence of liquid 1-chloroalkane viscosity // High Temperatures. 2016. V. 54. P. 872.