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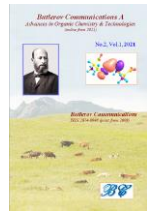

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Numerical characterization of the structure of an organic molecule. Part 20. Relationship between the acentric factor and the structural-mass parameter in the series of *n*-alkanes and 1-halogen-*n*-alkanes

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Abstract

On the example of a number of alkanes of normal structure, as well as a number of 1-halogen-*n*-alkanes, further research is carried out on the features of the relationship between the physical and chemical properties of organic compounds with the work of molar mass on the value of the topological index of Wiener in the degree 2/3. This value is considered as a characteristic of the moment of inertia of the rotational movement of molecules and is in a correlation with almost all the physical and chemical properties of nonelectrolytes in the liquid phase. Linear "structure-property" correlations, characterized by high correlation ratio values, are performed when used as an argument of innumerable degrees of the said work. The peculiarity of the structure of molecules *n*-alkanes and 1-halogen-*n*-alkanes is their topological-structural identity. This phenomenon is called "isotopology." The principle of thermodynamic similarity is allowed for isotope systems. One of the defining numbers of the theory of thermodynamic similarity is the acentric factor of Pitzer. The proposed paper examines the relationship between the Pitzer acentric factor, as well as the melting points and enthalpy of vaporization, the compounds considered to be the work of molar mass to the value of the topological Wiener index at 2/3. The indicated value in the degree ¼ correlates with the acentric factor of the series of *n*-alkanes, as well as 1-bromine, 1-fluorine, and 1-chloro-*n*-alkanes. At the same time, each set of homologies forms its own dependence. However, the introduction of degree adjustments based on the ratio of electronic energies to alkanes and isotopologic 1-halogen-*n*-alkanes provides a general

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dependence covering the entire dataset of the compounds under consideration. Similarly, two common dependences have been obtained for the melting temperature of the compounds considered with even and odd number of atoms in the skeletons of molecules, including heteroatom. The possibility of constructing general dependences by introducing corrections was used to predict the enthalpy of vaporization of some halogenated alkanes for which experimental data have not been established, which indicates that the proposed approach is promising.

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