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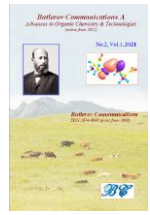

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Numerical characterization of the structure of an organic molecule. Part 22.

Relationship between a melting temperature and an enthalpy of vaporization of of 2- and 3-halogen-*n*-alkanes with a structure-mass parameter

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Abstract

We used non-integer powers of the product of the molar mass by the value of the topological Wiener index to the power of 2/3 (J_W) to prediction the physicochemical properties of organic compounds in the liquid phase by calculation. Topologically and structurally identical (isotopological) systems are considered, in particular *n*-alkanes and 1-halogen-*n*-alkanes. To calculate the melting points of 2- and 3-halogen-*n*-alkanes, the range of melting points of 2- and 3-methyl-*n*-alkanes has been expanded. We used for this the experimental data available in the literature on the values of this value for a number of methylsubstituted *n*-alkanes from those considered in this work. The obtained data, as well as the literature data, were used to calculate the values of the melting temperature of halogenated alkanes. The calculations were carried out taking into account the corrections calculated on the basis of the ratio of the atomization energies of isotopological halogenated alkanes and methylalkanes, since isotopology allows the principle of thermodynamic similarity to be fulfilled. The obtained values form four arrays of points, firstly, by the sign of 2- and 3-substitution, and secondly by the sign of parity. In this case each array is one straight line which is located below the graph of the melting point versus J_W in a non-integer degree for isotopological 2- and 3-methyl-*n*-alkanes. In contrast to the melting point, the enthalpy of vaporization is insensitive to the parity of carbon atoms; its feature is the closeness of values for isomers belonging to the same series and class. Taking this into account, on the basis of the statement on the

similarity of the properties of isotopological systems, the values of the enthalpy of vaporization of a number of 2- and 3-methyl-*n*-alkanes and 2- and 3-halogen-*n*-alkanes have been determined. The obtained values form a set of points corresponding to isomeric compounds, while a pronounced dependence on the mass of the substituent in the 2 and 3 positions is monitored. The enthalpy values change symbatically with the change in mass within a series. The set of dependences of the considered physical and chemical properties on the J_W values in non-integer powers makes it possible to use this parameter to systematize the properties of organic compounds.

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