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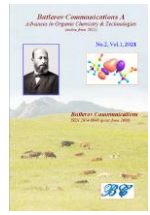

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Numerical characterization of the structure of an organic molecule. Part 21.

Acentric factor and structurally-mass parameter of the 2-, 3-methyl- and 2-, 3-halogen-*n*-alkanes

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Abstract

On the example of a series of 2- and 3-methyl-*n*-alkanes and 2- and 3-halogen-*n*-alkanes, where halogen is bromine, fluorine and chlorine, a study is underway of the possibility of using the product of the molar mass by the value of the Wiener topological index to the power of 2/3 (J_W) for predicting various physicochemical properties of organic compounds in the liquid phase. This value is considered as a topological characteristic of the moment of inertia of rotational motion, and its noninteger powers are in a linear correlation with the properties of organic compounds. The peculiarity of the structure of the molecules of 2- and 3-methyl-*n*-alkanes and 2- and 3-halogen-*n*-alkanes is their topological and structural identity. This phenomenon is called "isotopology". The principle of thermodynamic similarity is allowed for the isotopological systems. One of the defining numbers of the theory of thermodynamic similarity is the Pitzer acentric factor or the Pitzer acentric factor. Numerical values of the acentric factor can be calculated using data on critical pressure, critical temperature and boiling point. Calculations of the Pitzer factor values performed for a series of 2- and 3-methyl-*n*-alkanes correlate with the J_W values to the power of ¼. In this case each of the two sets of homologues forms its own dependence corresponding to substitutions in 2 and 3 positions. The 2- and 3-methyl-*n*-alkanes are systems isotopological to 2- and 3-halogen-*n*-alkanes. Accordingly, the principle of similarity must be fulfilled for these compounds. With this in mind, the corrections to the exponent JW of 2-, 3-halogen-*n*-alkanes were calculated based on the ratio of the atomization energy of alkyl-substituted alkanes to the atomization energy of halogen-substituted alkanes. Using the corrections for the considered alkyl halides, the values of the

critical pressure, critical temperature and boiling point were calculated, and then the acentric factor. The calculated values of the latter value form two data samples corresponding to 2-halogenated and 3-halogenated alkanes. Taking into account the corrections based on the ratio of the atomization energy, the general dependences of the acentric factor on J_W were obtained in a non-integer degree, including methylalkanes and haloalkanes, which is considered as evidence of the validity of the approach and the reliability of the results obtained.

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