

Thematic course: Numerical characteristics of the structure of organic molecules. Part 16.

Relationship of melting points of fluoro-, chloro-, and bromoderivatives of normal structure alkanes with moments of inertia of rotational motion

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Keywords: moment of inertia of the rotational movement, the topological index, melting and boiling points, halogenated alkanes.

Abstract

For the series of bromium-, fluoro- and chloro-derivatives of normal structure alkanes, the research has been carried out with correlation analysis of relationship of melting and boiling temperatures of the studied substances with characteristics of structures and components of inertia moment of rotational motion of molecules, as well as the new energy and structural parameter E_w (the ratio of the total electron energy (E) to the value of Wiener topological index to the 2/3 power).

The dependences of melting temperature and the boiling point of the substances in question on the characteristics of the structure and components of inertia moment of rotational motion of molecules, as well as on the energy and structural parameters indicate different forms of molecules at the phase transitions.