

Thematic course: Numerical characteristics of the structure of organic molecules. Part 15.

Relationship of melting points of normal structure alkanes with the energy characteristics of molecules

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Keywords: moment of inertia of the rotational movement, the topological index.

Abstract

For a number of normal structure alkanes, the relationship of melting and boiling points with characteristics of structures have been investigated, namely, the components of inertia moment of rotational motion as well as the HOMO energy. For a description of the melting point and the boiling point of the substances in question, we propose a new parameter, equal to the ratio of the total electron energy of alkanes to the value of Wiener topological index to the 2/3 power.