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Topological approach to the calculation of the heat capacity of the ultimate hydrocarbons

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Abstract

Research and simulation of the physical chemical properties of substances is a complex and urgent task. The heat capacity is an important thermophysical characteristic of the substance, which is often necessary for technological, scientific and engineering calculations. To date, not many methodologies for calculation this value have been proposed, but they are also not accurate enough.

The aim of this paper is to develop a topological model of the structure-property for an adequate calculation of the heat capacity of hydrocarbons. The adequacy of the model is confirmed by statistical data processing. Comparison of reference and calculated values of the property is shown, which shows the high adequacy of the proposed model. The results can be used in scientific and engineering calculations.

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