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QSPR model for the forecast of dynamic viscosity of arenas by the topological characteristics of molecules

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Abstract

Prediction of the dynamic viscosity of saturated hydrocarbons vapors is an important step in the calculation of various processes and apparatuses in chemical technology.

In order to quickly determine the dynamic viscosity without resorting to the use of expensive equipment, methods of mathematical modeling are currently used. To predict the dynamic viscosity of saturated arenas vapors, a nonlinear multivariate regression model QSPR is proposed.

The model associates with a dynamic viscosity a set of descriptors – the topological characteristics of molecular graphs: the Randic index, the Wiener index, and also the functions of the eigenvalues of the topological matrix of the molecule, which reflect the main structural and chemical factors, such as branching, length of the carbon skeleton and energy parameters of molecules, for example, Hückel's perturbation spectrum of molecules, as well as affecting dynamic viscosity.

The objects of research used arenas. The studied sample included 40 hydrocarbons of a number of arenas. The proposed model adequately describes the dynamic viscosity of saturated arenas vapors. The coefficient of determination of the model is 0.986. The average absolute and relative error for the test sample of HF is $-2.46 \cdot 10^{-7}$ cP and 1.83%, respectively.

The model is applicable for engineering and scientific forecasts of the dynamic viscosity of various saturated arenas vapors.

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