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Relationship of critical parameteres of liquid-vapour in phase transition and topological characteristics of aromatic hydrocarbons

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Abstract

Calculation of the critical parameters of the arenas, such as temperature, pressure, compressibility coefficient, etc., is necessary for engineering calculations in power engineering, pipeline transport, chemical technology, petrochemistry, and solving scientific problems. At present, more methods for calculating physical and chemical properties are known on the basis of structural molecular characteristics. Fundamental methods for estimating, based on the method of adding increments and critical parameters by their structural, information characteristics, as well as the theory of phase transitions. In addition, there is a group of methods that uses structural topological parameters of molecules – the QSPR model (Quantative Structure – Properties Relationship), which are in fact a mathematical reflection of the Butlerov theory of the influence of structures on the properties of organic substances.

Proposed nonlinear model for calculation of critical parameters (temperature, pressure and coefficient of compressibility) of arenes through topological characterisitics of molecular graph: Wiener's index, Randich's index and function of eigenvalues of topological matrix.

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