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Determining the Octanol-Water Partition Coefficient for Armchair Polyhex BN Nanotubes Using Topological Indices

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Abstract : The aim of this paper is to investigate theoretically and establish a predictive model for determination LogP of armchair polyhex BN nanotubes by using simple descriptors. The relationship between the octanol-water partition coefficient (LogP) and quantum chemical descriptors, electric moments, and topological indices of some armchair polyhex BN nanotubes with various lengths and fixed circumference are represented. Based on density functional theory (DFT) electric moments and physico-chemical properties of those nanotubes are calculated. The DFT method performed based on the Becke's 3-parameter formulation with the Lee-Yang-Parr functional (B3LYP) method and 3-21G standard basis sets. For the first time, the relationship between partition coefficient and different properties of polyhex BN nanotubes is investigated.

Keywords : topological indices, quantum descriptors, DFT method, nanotubes
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