

脂肪醛和脂肪酮的沸点与分子结构关系的拓扑化学研究

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摘要 根据分子拓扑学原理,通过采用信息量丰富的染色分子图代替隐氢图,借助于距离矩阵表征分子图中顶点的连接性和标识分子图中顶点性质的差异,发展了一种适用于含杂原子分子体系结构性能研究的新方法,

据此探讨了脂肪醛和脂肪酮的沸点与分子结构之间的关系,提出一个既能合理表征结构性能关系、又能预测沸点的定量关系式。结果表明,沸点预测值与实验值的一致性令人满意,平均误差0.21%。

关键词 [脂肪族醛](#) [脂肪族酮](#) [结构与性能关系](#) [分子结构](#) [沸点](#) [拓扑化学](#) [拓扑指数](#) [结构表征定量构效关系](#)

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Studies on the relationship between boiling points of aldehydes and alkanones and their molecular structures by using molecular topology

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Abstract Based on the molecular topology, the colored molecular graph is used to replace the hydrogen-suppressed graph, and distance matrix is used to characterize molecular structure and dyeing factors are proposed to distinguish the difference among the radicals in molecules, a new method, which can be used to study the structure property relationship of molecules containing heteroatoms, is developed. The method is used to study the relationship between boiling points and molecular structures of aldehydes and alkanones, and a quantitative relation that can be used to characterize the structure-property relationship and to predict the boiling points of aldehydes and alkanones is developed. The calculated results show that the predicted boiling points are in good agreement with the experimental data, and the mean relative deviation is 0.21%. Not only can the quantitative relation be used to predicted the boiling points of aldehydes and alkanones, but can help to understand the structure- property relationship of matter.

Key words [ALIPHATIC ALDEHYDES](#) [ALIPHATIC KETONES](#) [STRUCTURE AND PROPERTY CORRELATION](#) [MOLECULAR STRUCTURE](#) [BOILING POINTS](#) [STRUCTURE CHARACTERISTICS](#) [QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP](#)

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