计算烷烃沸点的新方法-基团键贡献法

王克强,王捷

洛阳师范学院化学系;许昌职业技术学院

摘要　　根据分子中基团的特性和连接性，将基团贡献法和化学键贡献法结合在一起，发展了一种直接根据分子结构信息计算烷烃沸点的新方法-基团键贡献法，此方法同时具有基团贡献法和化学键贡献法的特点。对753种烷烃(C2～C100)的计算结果表明，沸点计算值与实验值的一致性令人满意，平均误差0.46%。

关键词   烷烃   化学键贡献法   结构与性能关系   沸点   分子结构   基团贡献法   基团键贡献法

分类号   O621.16

A new group contribution method for calculating the boiling point of alkane

Wang Keqiang,Wang Jie

Abstract Based on characteristics and connectivity of groups in molecules, the group bonds can be applied to describe the molecular structure. The group bonds contained information of group property and connectivity in molecules. Group bonds, obtained directly from molecular structure, can be used to calculate properties of the molecules. A new method, the group contribution method, was developed to calculate the boiling points of alkanes based on the molecular structures. The calculated results showed that the calculated boiling points of alkanes were in good agreement with the experimental data, with a mean relative deviation of 0.46% for 753 alkanes (C2～C100). The group bond contribution method had advantages over the group contribution method and chemical bond contribution method.

Key words   ALKANE   STRUCTURE AND PROPERTY CORRELATION   BOILING POINTS   MOLECULAR STRUCTURE   GROUP CONTRIBUTION

DOI: