有机化学 2003 23 (10): 1169-1176 ISSN: 0567-7351 CN: 31-1320/06

用均根拓扑指数与路径数预测链烷烃的沸点和热力学性质

冯长君,王超

徐州师范大学化学系

收稿日期 修回日期 网络版发布日期 接受日期

摘要 以距离矩阵为基础，建构调和均根拓扑指数（K），以表征链烷烃分子的大小 和分支情况，85种链烷烃的沸点(T_b)、标准生成焓(Δ_rH_m~θ)、标准熵(S_m~θ)、标准生成自由能(Δ_fG_m~θ)与K及路径数(P_2, P_3)的回归方程为: ln(793- T_b) = 6.48346-0.10092K + 0.00131P_2-0.01110P_3, R = 0.9996; -Δ_fH_m~θ = 62.664 + 25.331 K + 6.597 P_2 - 0.678 P_3, R = 0.9984; S_m~θ = 170. 691 + 67.425 K - 4.712P_2 + 5.251 P_3, R = 0.9989; Δ_fG_m~θ = -45.677 + 10.060 K + 0.555 P_2 + 2.342P_3, R = 0.9935。它们的计算值与相应实验值都非常吻合。结果表明，K对链烷烃具有良好的结构选择性和性质相关性。

关键词 拓扑指数 烷烃 沸点 热力学性质 定量构效关系 自由能

分类号 0642

Predicting Boiling Points and Thermodynamic Properties for Alkanes with a Topological Index of Square Root of Harmonic Average and Numbers of Path

Feng Changjun,Wang Chao

Department of Chemistry, Xuzhou Normal University

Abstract A topological index (K) of square root of harmonic average based on the distance matrix, which can be used to characterize the size and branching for alkanes, is derived in this paper. Their regression models between the boiling points (T_b, K), thermodynamic properties such as the standard enthalpies (Δ_FH_m~θ, kJ·mol~(-1)) of formation, the standard entropies (S_m~θ, J·mol~(-1)·K~(-1)), the standard free energies (Δ_Fg_M~θ, Kj·mol~(-1)) of formation and K, numbers of path (such as P_2, P_3) are established as following: (1) In(793 - T_b) = 6.48346 - 0.10092K + 0.00131P_2-0.01110P_3, R=0.9996; (2) -Δ_FH_m~θ = 62.664 + 25.331K + 6.597 P_2 - 0.678P_3, R=0.9984; (3)S_m~θ= 170.691 +67.425K-4.712P_2 + 5.251P_3, R = 0.9989; (4) Δ _Fg_m~θ= - 45.677 + 10.060K + 0.555 P_2 + 2.342P_3, R = 0.9935. The calculated values are all obtained in good agreement with experimental data by above models. It is concluded that the novel index bears good structural selectivity and property relativity.

Key words topological index ALKANE BOILING POINTS THERMODYNAMIC PROPERTIES QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP FREE ENERGY

DOI:

通讯作者