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本刊中 包含“分子连接性指数”的相关文章

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分子连接性指数~mX~z与不饱和链烃沸点的定量关系研究

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摘要 提出了一个计算分子中成键原子点价δ_i~z的新方法，以δ_i~z为基础建构的新的分子连接性指数为~mX~z = ∑(δ_i~z·δ_j~z·δ_k~z…)~(-0.5)，其中 ~0X~z，~1X~z的定义为：~0X~z = ∑(δ_i~z)~(-0.5), ~1X~z = ∑(δ_i~z·δ _j~z)~(-0.5)，并研究了~0X~z,~1X~z与不饱和链烃沸点的相关性。结果表明，该 拓扑指数具有良好的结构-性质相关性。以~0X~z,~1X~z和碳原子数N为结构参数分 别与80个单烯烃、39个单炔烃、169个不饱和链烃（包括烷烃、炔烃及烯炔）的沸 点进行关联所得到的三元回归方程为：单烯烃，log(779.13-bp) = 2.822433-0. 0133346 ~0X~z - 0.0638379 ~1X~2 + 0.0111229N (R = 0.99895, F = 202783. 65, s = 3.36)；单炔烃，log(797.47-bp) = 2.809912-0.0108374~0X~z - 0. 0864540 ~1X~z + 0.0233028N (R = 0.99935, F = 98657.36, s = 3.65);不饱和 链烃，log(741.26-bp) = 2.779526 + 0.0194388~0X~z - 0.0519158~1X~z - 0. 0211047N (R = 0.99467, F = 82387.26, s = 7.74)。应用这些经验公式可以预测 不饱和链烃的沸点。

关键词 分子连接性指数 沸点 烯烃 烷烃 炔烃

分类号 0621

Study on Quantitative Structure-Property Relationship between Molecular Connectivity Index (~mX~z) and Boiling Points of Aliphatic Unsaturated Hydrocarbons

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Abstract In this paper, a new method of calculating delta (δ_i~z) of bonding atoms in molecules is proposed. Based on the δ_i~z a novel molecular connectivity index ~mX~z is set up as ~mX~z = ∑(δ_i~z·δ _j~z·δ_k~z…)~(-0.5), in which ~0X~z amd ~1X~z are defined as ~0X~z = ∑(δ_i~z)~(-0.5) and ~1X~z = ∑(δ_i~z·δ_j~z)~(-0.5) . Correlation between the~0X~z, ~1X~z and the boiling points for aliphatic unsaturated hydrocarbons is studied. The results show that the topological index has good structure-property correlativity. Relationships between the three molecular structure parameters of Xz, Xz and N (N refers to the number of carbon atoms in molecules), and the boiling points for 80 alkenes, 39 alkynes and 169 aliphatic unsaturated hydrocarbons were examined, respectively, and the following three variable regression equations were obtained: for alkenes, log(779.13 - bp) = 2.822433 - 0.0133346 ~0X~z - 0.0638379 ~1X~z + 0.0111229 N (R = 0.99895, F = 202783.65, s=3.36); for alkynes, log(797.47 - bp) = 2.809912 - 0.0108374 ~0X~z - 0.0864540 ~1X~z+ 0. 02330287V (R = 0.99935, F = 98657.36, s = 3.65); and for aliphatic unsaturated hydrocarbons, log (741.26 -bp)= 2.779526 + 0.0194388 ~0X~z- 0.0519158 ~1Z~z-0.0211047 N (K=0.99467, F = 82387.26, s = 7.74) . These experimental formulae can be used to predict the boiling points of the hydrocarbons.

Key words molecular connectivity index BOILING POINTS ALKENE ALKANE ALKYNE

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