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RESEARCH NOTES

用对应态基团贡献法估算有机物偏心因子

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摘要 A new estimation method was proposed by combining the corresponding state principle with the group contribution method through introducing the concept of assumed-critical properties. Combining it with the Reidel equation, a new acentric factor correlation equation（CSGC-Reidel）was developed. Contribution values of 70 groups were obtained by correlating acentric factor data of 228 organic compounds of 14 type substances including saturated hydrocarbons, unsaturated hydrocarbons, cyclanes, aromatics, oxygen compounds, nitrogen compounds, halohydrocarbons, etc. The average error of acentric factor is 3.52% between the literature data and the predicated with the new estimation method.

关键词 对应态基团贡献法; 估算方法; 性质测定; 有机物; 偏心因子;
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Estimation of Acentric Factor of Organic Compounds with Corresponding States Group Contribution Method

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Abstract A new estimation method was proposed by combining the corresponding state principle with the group contribution method through introducing the concept of assumed-critical properties. Combining it with the Reidel equation, a new acentric factor correlation equation（CSGC-Reidel）was developed. Contribution values of 70 groups were obtained by correlating acentric factor data of 228 organic compounds of 14 type substances including saturated hydrocarbons, unsaturated hydrocarbons, cyclanes, aromatics, oxygen compounds, nitrogen compounds, halohydrocarbons, etc. The average error of acentric factor is 3.52% between the literature data and the predicated with the new estimation method.

Key words acentric factor; estimation of properties; corresponding state group contribution（CSGC）; Edmister equation; Reidel equation

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