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预测纯流体表面张力的一个新模型

杨春生, 仲崇立

Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, China

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摘要 A new model based on the theoretical work of Boudh-Hir and Mansoori was developed for
prediction of surface tension of pure fluids. The new model has the advantage of not requiring densities in the calculation, and the input parameters are critical temperature and connectivity indices. A total of 209 compounds covering a wide variety of substances were used to develop the model, and the overall correlative AAD is 4.21%. To test its predictive ability, the model is further used to predict the surface tension of 25 more compounds that were not included in the model development. The overall predictive AAD is 4.07%, which illustrates that the model is reliable. The model proposed is simple and easy to apply, with good predictive accuracy.

关键词 connectivity index critical temperature Gibbs free energy surface tension pure fluid

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A New Model for Prediction of Surface Tension of Pure Fluids

YANG Chunsheng, ZHONG Chongli

Department of Chemical Engineering, Beijing University of Chemical Technology, Beijing
100029, China

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Abstract A new model based on the theoretical work of Boudh-Hir and Mansoori was developed for prediction of surface tension of pure fluids. The new model has the advantage of not requiring densities in the calculation, and the input parameters are critical temperature and connectivity indices. A total of 209 compounds covering a wide variety of substances were used to develop the model, and the overall correlative AAD is 4.21%. To test its predictive ability, the model is further used to predict the surface tension of 25 more compounds that were not included in the model development. The overall predictive AAD is 4.07%, which illustrates that the model is reliable. The model proposed is simple and easy to apply, with good predictive accuracy.

Key words connectivity index; critical temperature; Gibbs free energy; surface tension; pure fluid

通讯作者:
杨春生
作者个人主页: 杨春生; 仲崇立