

عنوان مقاله:

TOWARD A PREDICTIVE MODEL FOR ESTIMATING CRITICAL PROPERTIES OF PURE COMPONENTS

محل انتشار:

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خلاصه مقاله:

In this study, least square support vector machine (LSSVM) is utilized to predict and calculate critical properties including the critical pressure, temperature and volume of pure compounds. The datasets of 563 compounds from various chemical groups containing: paraffins; cycloparaffins; monooleffins and dioleffins; cyclooleffins and actylens; benzene derivatives; condensed ring aromatics and derivatives; acids, alcohols, and phenols and aldehydes; amines and nitrogen containing components; esters; ethers, ketones; halogenated hydrocarbons; sulfur containing hydrocarbons have been used to propose a comprehensive non-group contribution predictive model. The parameters of the model are optimized through a robust optimization tool named coupled simulated annealing (CSA). The developed model gives more accurate predictions compared to previously proposed methods. Using this robust method, average absolute percent relative error obtained 5.92% for critical pressure, 1.37% for critical temperature and 2.98% for critical volume.

کلمات کلیدی:

Critical properties; non-group contribution; least square support vector machine

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