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Estimating the density of deep eutectic solvents applying supervised machine learning techniques (/paperRedirect/1506706873396346880)

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Deep eutectic solvents (DES) are recently synthesized to cover limitations of conventional solvents. These green solvents have wide ranges of potential usages in real-life applications. Precise measuring or accurate estimating thermophysical properties of DESs is a prerequisite for their successful applications. Density is likely the most crucial affecting characteristic on the solvation ability of DESs. This study utilizes seven machine learning techniques to estimate the density of 149 deep eutectic solvents. The density is anticipated as a function of temperature, critical pressure and temperature, and acentric factor. The LSSVR (least-squares support vector regression) presents the highest accuracy among 1530 constructed intelligent estimators. The LSSVR predicts 1239 densities with the mean absolute percentage error (MAPE) of 0.26% and $R^2 = 0.99798$. Comparing the LSSVR and four empirical correlations revealed that the earlier possesses the highest accuracy level. The prediction accuracy of the LSSVR (i.e., MAPE = 0.26%) is 74.5% better than the best-obtained results by the empirical correlations (i.e., MAPE = 1.02%).

中文翻译:

中文翻译由计算机程序完成, 如与英文原文有差异, 以后者为准

应用监督机器学习技术估计深共熔溶剂的密度

最近合成了深共熔溶剂 (DES), 以弥补传统溶剂的局限性。这些绿色溶剂在实际应用中具有广泛的潜在用途。精确测量或准确估计 DES 的热物理性质是其成功应用的先决条件。密度可能是影响 DES 溶剂化能力的最关键特征。本研究利用七种机器学习技术来估计 149 种深共熔溶剂的密度。预计密度是温度、临界压力和温度以及无心因素的函数。LSSVR (最小二乘支持向量回归) 在 1530 个构建的智能估计器中表现出最高的准确度。LSSVR 预测 1239 个密度, 平均绝对百分比误差 (MAPE) 为 0.26%, $R^2 = 0.99798$ 。比较 LSSVR 和四个经验相关性表明, 较早的具有最高的准确度水平。LSSVR 的预测精度 (即 MAPE = 0.26%) 比经验相关性获得的最佳结果 (即 MAPE = 1.02%) 好 74.5%。

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