

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 12.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.96e-01

Confidence level: 5.76e-01

Nearest Neighbors from the Training Set

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1-Butanol

Measured: 3.16

Predicted: 8.95

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Butylamine

Measured: 75.9

Predicted: 19.9

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1-Propanol

Measured: 3.02

Predicted: 4.69

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Pyridine

Measured: 39.8

Predicted: 20.1

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1,2-Diethylhydrazine

Measured: 15.1

Predicted: 14.1