

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: 3770 L/kg

Global applicability domain: Outside

Local applicability domain index: 4.31e-01

Confidence level: 7.94e-01

Nearest Neighbors from the Training Set

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3,4,5,6-Tetrachloroguaiacol

Measured: 708

Predicted: 685

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2,3,4,5-Tetrachloronitrobenzene

Measured: 17000

Predicted: 14600

Image not found

2,3,5,6-Tetrachloronitrobenzene

Measured: 11200

Predicted: 12600

Image not found

4,5,6-Trichloroguaiacol

Measured: 631

Predicted: 134

Image not found

Pentachloronitrobenzene

Measured: 9550

Predicted: 10500