

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.37e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.79e-01

Confidence level: 7.48e-01

Nearest Neighbors from the Training Set

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Molinate

Measured: 5.18e-03

Predicted: 3.37e-03

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EPTC

Measured: 1.98e-03

Predicted: 1.25e-03

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Ethiolate

Measured: 2.03e-02

Predicted: 2.19e-02

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Vernolate

Measured: 4.43e-04

Predicted: 4.86e-04

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Pebulate

Measured: 4.92e-04

Predicted: 4.82e-04