

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: 10.8 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.42e-01

Confidence level: 8.27e-01

Nearest Neighbors from the Training Set

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Morpholine

Measured: 11.5

Predicted: 10.8

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4-Methylmorpholine

Measured: 9.89

Predicted: 9.71

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N-Nitrosomorpholine

Measured: 8.61

Predicted: 9.55

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1-Methylimidazole

Measured: 12.2

Predicted: 7.43

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N-Ethylmorpholine

Measured: 8.68

Predicted: 6.40