

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: 9.51e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.02e-01

Confidence level: 5.27e-01

Nearest Neighbors from the Training Set

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HFC-41

Measured: 6.67e-01

Predicted: 9.51e-01

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HFC-161

Measured: 4.49e-02

Predicted: 1.72e-01

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Acetaldehyde

Measured: 22.7

Predicted: 13.1

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Propanal

Measured: 5.27

Predicted: 3.91

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Acetone

Measured: 17.2

Predicted: 6.59