

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: 9.23e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.97e-01

Confidence level: 8.05e-01

Nearest Neighbors from the Training Set

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Octane

Measured: 5.78e-06

Predicted: 9.23e-06

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1-Nonene

Measured: 8.87e-06

Predicted: 6.62e-06

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2,3,4-Trimethylpentane

Measured: 2.01e-05

Predicted: 1.15e-05

[Image not found](#)

1-Octene

Measured: 3.65e-05

Predicted: 3.95e-05