

2,2,3-Trimethylbutane
464-06-2 | DTXSID7060047

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: 4.67e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.38e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

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Pentane, 2,2-dimethyl-

Measured: 4.39e-05

Predicted: 4.70e-05

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Pentane,3,3-dimethyl-

Measured: 5.91e-05

Predicted: 4.77e-05

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2,4-Dimethylpentane

Measured: 5.49e-05

Predicted: 4.61e-05

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2-Methylhexane

Measured: 2.53e-05

Predicted: 4.32e-05