

Nonene
27215-95-8 | DTXSID6027927

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: 6.90e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.07e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

Image not found

1-Nonene

Measured: 8.87e-06

Predicted: 6.62e-06

Image not found

1-Bromooctane

Measured: 8.65e-06

Predicted: 1.03e-05

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Octane

Measured: 5.78e-06

Predicted: 9.23e-06

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1,1,3-Trimethylcyclohexane

Measured: 1.40e-05

Predicted: 7.65e-06

Image not found

Nonane

Measured: 1.72e-06

Predicted: 1.93e-06