

Nonane

111-84-2 | DTXSID9025796

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: 1.93e-06 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.97e-01

Confidence level: 6.91e-01

Nearest Neighbors from the Training Set

Image not found

Nonane

Measured: 1.72e-06

Predicted: 1.93e-06

Image not found

4-Methyloctane

Measured: 8.97e-07

Predicted: 2.19e-06

Image not found

1-Decene

Measured: 4.06e-06

Predicted: 2.00e-06

Image not found

1-Nonene

Measured: 8.87e-06

Predicted: 6.62e-06

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Cyclopentane, pentyl-

Measured: 8.20e-07

Predicted: 1.76e-06