

Nitroethane
79-24-3 | DTXSID8020969

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.07e-03

Global applicability domain: Inside

Local applicability domain index: 5.84e-01

Confidence level: 5.06e-01

Nearest Neighbors from the Training Set

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Nitroethane

Measured: 0.18

Predicted: 3.07e-03

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Acetaldehyde oxime

Measured: -0.130

Predicted: 2.71e-01

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1-Nitropropane

Measured: 0.87

Predicted: 9.14e-01

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Glycine

Measured: -3.21

Predicted: -2.61

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2-Nitropropane

Measured: 0.93

Predicted: 1.03