

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.25

Global applicability domain: Inside

Local applicability domain index: 9.63e-01

Confidence level: 6.54e-01

Nearest Neighbors from the Training Set

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Nitroethane

Measured: 2.88

Predicted: 2.25

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Butane

Measured: 1.53

Predicted: 2.22

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Dichloromethane

Measured: 2.27

Predicted: 2.41

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Methyl acetate

Measured: 2.31

Predicted: 2.41

[Image not found](#)

Ethyl formate

Measured: 2.19

Predicted: 2.41