

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 14.4 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.74e-01

Confidence level: 7.30e-01

Nearest Neighbors from the Training Set

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Methyl acetate

Measured: 20.8

Predicted: 198

[Image not found](#)

Dichloroacetic acid

Measured: 17.2

Predicted: 2.06e-01

[Image not found](#)

Dimethylaminoethanol

Measured: 10.1

Predicted: 2.33

[Image not found](#)

2,3-Dimethylbutan-2-ol

Measured: 12.0

Predicted: 5.17

[Image not found](#)

Dichlorvos

Measured: 2.70

Predicted: 2.14e-02