

Isobutyl nitrite
542-56-3 | DTXSID3020750

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: 2.09 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.45e-01

Confidence level: 7.05e-01

Nearest Neighbors from the Training Set

[Image not found](#)

3-Mercaptopropanoic acid

Measured: 5.10

Predicted: 5.30e-02

[Image not found](#)

N-Methylcarbamic acid, ethyl ester

Measured: 8.92e-01

Predicted: 1.51

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Diethoxymethane

Measured: 3.97

Predicted: 50.4

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2,4-Pentanedione

Measured: 1.36

Predicted: 3.07

[Image not found](#)

1,3-Diethylbenzene

Measured: 7.80e-01

Predicted: 9.75e-01