

Propane, 2-methyl-1-nitro-
625-74-1 | DTXSID90211547

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: 7.40 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.34e-01

Confidence level: 8.27e-01

Nearest Neighbors from the Training Set

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Ethyl methyl sulfide

Measured: 6.88

Predicted: 121

[Image not found](#)

Ethyl 2-bromoisobutyrate

Measured: 7.79

Predicted: 3.11

[Image not found](#)

2,3-Dimethylbutan-2-ol

Measured: 12.0

Predicted: 5.17

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Ether, isobutyl methyl

Measured: 3.79

Predicted: 201

[Image not found](#)

Dimethylaminoethanol

Measured: 10.1

Predicted: 2.33