

Propane, 2-methyl-2-nitro-
594-70-7 | DTXSID0060488

Model Performance

Model	Data
-------	------

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: 9.73 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.41e-01

Confidence level: 8.11e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2,3-Dimethylbutan-2-ol

Measured: 12.0

Predicted: 5.17

[Image not found](#)

Ether, isobutyl methyl

Measured: 3.79

Predicted: 201

[Image not found](#)

Dimethylaminoethanol

Measured: 10.1

Predicted: 2.33

[Image not found](#)

Dichloroacetic acid

Measured: 17.2

Predicted: 2.06e-01

[Image not found](#)

Ethyl 2-bromoisobutyrate

Measured: 7.79

Predicted: 3.11