

Dimethylglyoxime
95-45-4 | DTXSID2044393

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: 2.71 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.74e-01

Confidence level: 5.29e-01

Nearest Neighbors from the Training Set

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Propane, 2-methyl-2-nitro-

Measured: 16.9

Predicted: 9.73

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Dimethylaminoethanol

Measured: 10.1

Predicted: 2.33

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Ether, isobutyl methyl

Measured: 3.79

Predicted: 201

[Image not found](#)

Diphenyl disulfide

Measured: 6.00e-02

Predicted: 1.73e-04

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2,3,3-Trimethyl-1-pentene

Measured: 3.10

Predicted: 35.2