

2-Butanone oxime
96-29-7 | DTXSID1021821

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: 35.0 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.08e-01

Confidence level: 5.14e-01

Nearest Neighbors from the Training Set

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Cyclopentane

Measured: 45.5

Predicted: 252

[Image not found](#)

1-Hexanethiol

Measured: 17.6

Predicted: 6.13

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Benzo[b]naphtho[2,1-d]thiophene

Measured: 132

Predicted: 4.00e-07

[Image not found](#)

HFC-152

Measured: 348

Predicted: 2760

[Image not found](#)

N-Nitrosodiethylamine

Measured: 8.60e-01

Predicted: 1.48