

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.72e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.79e-01

Confidence level: 5.26e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitrobutane

Measured: 1.50e-12

Predicted: 1.21e-12

Image not found

N-Butylnitrite

Measured: 2.72e-12

Predicted: 1.86e-12

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1-Nitropropane

Measured: 4.40e-13

Predicted: 5.94e-13

Image not found

2-Nitropropane

Measured: 2.60e-13

Predicted: 3.96e-13

Image not found

Dimethyl sulfoxide

Measured: 6.20e-11

Predicted: 1.83e-11