

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 9.88e-13 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.30e-01

Confidence level: 7.46e-01

Nearest Neighbors from the Training Set

Image not found

Diethyl sulfate

Measured: 1.80e-12

Predicted: 1.55e-12

Image not found

1-Nitropropane

Measured: 4.40e-13

Predicted: 5.94e-13

Image not found

1-Nitrobutane

Measured: 1.50e-12

Predicted: 1.21e-12

Image not found

2-Nitropropane

Measured: 2.60e-13

Predicted: 3.96e-13

Image not found

N-Butylnitrite

Measured: 2.72e-12

Predicted: 1.86e-12