

3-Methyl-1-nitrobutane
627-67-8 | DTXSID90211769

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: 1.97e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.57e-01

Confidence level: 7.98e-01

Nearest Neighbors from the Training Set

Image not found

Amyl nitrate

Measured: 3.14e-12

Predicted: 2.43e-12

Image not found

1-Nitrobutane

Measured: 1.50e-12

Predicted: 1.21e-12

Image not found

1-Propanol, 2,2-dimethyl-, nitrate

Measured: 8.50e-13

Predicted: 1.32e-12

Image not found

Isoamyl nitrate

Measured: 1.85e-12

Predicted: 1.87e-12