

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

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.24e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.10e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitrobutane

Measured: 4.46e-02

Predicted: 6.99e-02

Image not found

2-Nitropropane

Measured: 2.15e-01

Predicted: 2.16e-01

Image not found

1-Nitropropane

Measured: 1.68e-01

Predicted: 2.14e-01