

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 156 °C

Global applicability domain: Inside

Local applicability domain index: 6.71e-01

Confidence level: 7.92e-01

Nearest Neighbors from the Training Set

Image not found

3-Methyl-1-nitrobutane

Measured: 164

Predicted: 156

Image not found

1-Nitrobutane

Measured: 153

Predicted: 144

Image not found

2-Nitrobutane

Measured: 140

Predicted: 140

Image not found

Propane, 2-methyl-1-nitro-

Measured: 141

Predicted: 140

Image not found

1-Chloro-1-nitropropane

Measured: 142

Predicted: 152