

1-Nitrobutane

627-05-4 | DTXSID8020967

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 144 °C

Global applicability domain: Inside

Local applicability domain index: 8.74e-01

Confidence level: 8.35e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Nitrobutane

Measured: 153

Predicted: 144

[Image not found](#)

Propane, 2-methyl-1-nitro-

Measured: 141

Predicted: 140

[Image not found](#)

2-Nitrobutane

Measured: 140

Predicted: 140

[Image not found](#)

Propane, 2-methyl-2-nitro-

Measured: 127

Predicted: 135

[Image not found](#)

1-Chloro-1-nitropropane

Measured: 142

Predicted: 152