

1-Chloro-1-nitropropane
600-25-9 | DTXSID2024797

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: 152 °C

Global applicability domain: Inside

Local applicability domain index: 8.70e-01

Confidence level: 7.27e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Chloro-1-nitropropane

Measured: 142

Predicted: 152

[Image not found](#)

1-Chloro-2-nitropropane

Measured: 173

Predicted: 162

[Image not found](#)

1,1-Dichloro-1-nitroethane

Measured: 124

Predicted: 136

[Image not found](#)

1-Nitrobutane

Measured: 153

Predicted: 144