

2-Nitropropane
79-46-9 | DTXSID6020981

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: 124 °C

Global applicability domain: Inside

Local applicability domain index: 7.01e-01

Confidence level: 8.24e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Nitropropane

Measured: 120

Predicted: 124

[Image not found](#)

1-Nitropropane

Measured: 131

Predicted: 129

[Image not found](#)

Propane, 2-methyl-2-nitro-

Measured: 127

Predicted: 135

[Image not found](#)

1-Propene, 3-nitro-

Measured: 128

Predicted: 125