

2-Nitrobenzamide
610-15-1 | DTXSID0025733

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: 310 °C

Global applicability domain: Inside

Local applicability domain index: 3.42e-01

Confidence level: 7.09e-01

Nearest Neighbors from the Training Set

Image not found

2-Nitrobenzamide

Measured: 317

Predicted: 310

Image not found

3-Nitrobenzamide

Measured: 313

Predicted: 310

Image not found

2-Aminobenzamide

Measured: 300

Predicted: 299

Image not found

4-Aminoacetanilide

Measured: 267

Predicted: 290

Image not found

N-(2-Methoxyphenyl)acetamide

Measured: 304

Predicted: 301