

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 169 °C

Global applicability domain: Inside

Local applicability domain index: 9.15e-01

Confidence level: 5.72e-01

Nearest Neighbors from the Training Set

Image not found

2-Nitrobenzamide

Measured: 177

Predicted: 169

Image not found

3-Nitrobenzamide

Measured: 143

Predicted: 167

Image not found

4-Nitrobenzamide

Measured: 200

Predicted: 173

Image not found

2-Chloro-4-nitrobenzamide

Measured: 172

Predicted: 173

Image not found

Acetamide, N-(2-nitrophenyl)-

Measured: 94.0

Predicted: 122