

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.20e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.38e-01

Confidence level: 5.30e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2,2-Dibromo-3-nitrilopropionamide

Measured: 6.20e-02

Predicted: 1.07e-01

[Image not found](#)

Isosorbide dinitrate

Measured: 2.33e-03

Predicted: 4.44e-03

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2,2,2-Tribromoacetamide

Measured: 5.41e-02

Predicted: 5.67e-02

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2,2-Dibromoacetamide

Measured: 8.76e-02

Predicted: 1.47e-01