

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.22e-01

Global applicability domain: Inside

Local applicability domain index: 7.97e-01

Confidence level: 6.62e-01

Nearest Neighbors from the Training Set

Image not found

2-Nitrobenzamide

Measured: -0.120

Predicted: 3.22e-01

Image not found

4-Nitrobenzamide

Measured: 0.82

Predicted: 3.28e-01

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3-Nitrobenzamide

Measured: 0.77

Predicted: 3.15e-01

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2,4-Diaminobenzoic acid

Measured: -0.310

Predicted: -0.534

Image not found

3,4-Diaminobenzoic acid

Measured: 0.13

Predicted: -0.508