

2-Nitrobutane
600-24-8 | DTXSID3020968

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.81

Global applicability domain: Inside

Local applicability domain index: 9.87e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

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Tetrahydrofuran

Measured: 2.86

Predicted: 2.94

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1,2-Dichloroethane

Measured: 2.78

Predicted: 2.81

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Butanenitrile

Measured: 3.12

Predicted: 2.80

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Ethane, iodo-

Measured: 2.59

Predicted: 2.80

[Image not found](#)

1,1,1-Trichloroethane

Measured: 2.70

Predicted: 2.79