

1-Nitrobutane

627-05-4 | DTXSID8020967

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1.34

Global applicability domain: Inside

Local applicability domain index: 5.84e-01

Confidence level: 6.21e-01

Nearest Neighbors from the Training Set

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1-Pentanol

Measured: 0.7

Predicted: 8.64e-01

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Toluene

Measured: 2.07

Predicted: 1.94

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Anisole

Measured: 1.54

Predicted: 1.84

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Resorcinol

Measured: 0.98

Predicted: 1.45

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Phenol

Measured: 1.43

Predicted: 1.76