

N-ButylNitrite
544-16-1 | DTXSID8049418

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: 2.79

Global applicability domain: Inside

Local applicability domain index: 9.92e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

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1,1,1-Trichloroethane

Measured: 2.70

Predicted: 2.79

Image not found

Carbon tetrachloride

Measured: 2.79

Predicted: 2.78

Image not found

Ethane, iodo-

Measured: 2.59

Predicted: 2.80

Image not found

Butanenitrile

Measured: 3.12

Predicted: 2.80

Image not found

1,2-Dichloroethane

Measured: 2.78

Predicted: 2.81