

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.27e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.03e-01

Confidence level: 5.47e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Butyl vinyl ether

Measured: 3.00e-02

Predicted: 4.81e-02

[Image not found](#)

Vinyl isobutyl ether

Measured: 3.00e-02

Predicted: 5.20e-02

[Image not found](#)

1-Propene, 3,3'-oxybis-

Measured: 9.54e-01

Predicted: 6.49e-01

[Image not found](#)

2-Methoxyprop-1-ene

Measured: 13.9

Predicted: 2.31