

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.87

Global applicability domain: Inside

Local applicability domain index: 3.62e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

Image not found

2-Butanone oxime

Measured: 5.01

Predicted: 5.34

Image not found

Cyclohexane

Measured: 83.2

Predicted: 59.1

Image not found

Piperidine, 1-methyl-

Measured: 4.47

Predicted: 5.88

Image not found

cis-Nanophine

Measured: 5.01

Predicted: 6.12

Image not found

Furan

Measured: 5.01

Predicted: 4.88