

Butyl nitrate
928-45-0 | DTXSID70239143

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: 6.38

Global applicability domain: Inside

Local applicability domain index: 6.04e-01

Confidence level: 8.77e-01

Nearest Neighbors from the Training Set

Image not found

2-Nitropropane

Measured: 8.32

Predicted: 7.41

Image not found

2-Butanone oxime

Measured: 5.01

Predicted: 5.34

Image not found

Furan

Measured: 5.01

Predicted: 4.88

Image not found

Thiophene

Measured: 8.91

Predicted: 6.68

Image not found

Diethyl ether

Measured: 5.37

Predicted: 4.72