

2-Butanone oxime
96-29-7 | DTXSID1021821

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 135 °C

Global applicability domain: Inside

Local applicability domain index: 6.75e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

Image not found

2-Butanone oxime

Measured: 153

Predicted: 135

Image not found

Butanal oxime

Measured: 154

Predicted: 145

Image not found

Propyl isocyanate

Measured: 83.5

Predicted: 89.1

Image not found

Isopropyl nitrite

Measured: 40.0

Predicted: 68.9

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1-Nitropropane

Measured: 131

Predicted: 129