

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -2.05 °C

Global applicability domain: Inside

Local applicability domain index: 7.81e-01

Confidence level: 4.97e-01

Nearest Neighbors from the Training Set

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2-Butanone oxime

Measured: -29.5

Predicted: -2.05

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Butanal oxime

Measured: -29.5

Predicted: -4.19

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tert-Butyl isocyanate

Measured: 85.5

Predicted: 49.5

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Acetoxime

Measured: 61.0

Predicted: 37.2