

Paraldehyde
123-63-7 | DTXSID9023419

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: 16.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.57e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

Image not found

Paraldehyde

Measured: 12.6

Predicted: 16.3

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1,3,5-Trioxane

Measured: 60.2

Predicted: 46.2

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1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane

Measured: -30.0

Predicted: -17.6

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1,3,5-Trimethoxybenzene

Measured: 54.5

Predicted: 51.0

Image not found

1,4-Dioxane

Measured: 11.8

Predicted: -12.0