

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 6.15 days

Global applicability domain: Outside

Local applicability domain index: 2.37e-01

Confidence level: 8.68e-01

Nearest Neighbors from the Training Set

Image not found

Pentane

Measured: 40.7

Predicted: 6.52

Image not found

n-Hexane

Measured: 157

Predicted: 7.45

Image not found

Pentane, 2,2-dimethyl-

Measured: 88.3

Predicted: 6.21

Image not found

Heptane

Measured: 88.3

Predicted: 7.54

Image not found

Pentane, 3-ethyl-

Measured: 24.3

Predicted: 5.29