

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 139 °C

Global applicability domain: Inside

Local applicability domain index: 7.48e-01

Confidence level: 7.75e-01

Nearest Neighbors from the Training Set

Image not found

Paraldehyde

Measured: 124

Predicted: 139

Image not found

1-Propanol, 3-chloro-, acetate

Measured: 164

Predicted: 154

Image not found

Propyl chloroacetate

Measured: 161

Predicted: 154