

Cyclohexanol
108-93-0 | DTXSID4021894

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: 154 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 8.20e-01

Nearest Neighbors from the Training Set

Image not found

Cyclohexanol

Measured: 161

Predicted: 154

Image not found

Cyclopentanemethanol

Measured: 163

Predicted: 155

Image not found

trans-2-Methylcyclopentan-1-ol

Measured: 150

Predicted: 150

Image not found

1-Methylcyclopentanol

Measured: 136

Predicted: 148