

Cyclohexanol
108-93-0 | DTXSID4021894

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.72

Global applicability domain: Inside

Local applicability domain index: 8.95e-01

Confidence level: 5.73e-01

Nearest Neighbors from the Training Set

Image not found

Cyclohexanol

Measured: 5.18

Predicted: 4.72

Image not found

1-Hexanol

Measured: 5.18

Predicted: 4.67

Image not found

Dipropylamine

Measured: 3.59

Predicted: 4.37

Image not found

Piperidine

Measured: 4.04

Predicted: 4.32

Image not found

1-Pentanol

Measured: 4.69

Predicted: 4.17