

Isophorone
78-59-1 | DTXSID8020759

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: 7.87 °C

Global applicability domain: Inside

Local applicability domain index: 8.68e-01

Confidence level: 4.51e-01

Nearest Neighbors from the Training Set

Image not found

Isophorone

Measured: -8.10

Predicted: 7.87

Image not found

Cyclohexanone, 4-methyl-

Measured: -40.6

Predicted: -15.0