

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 207 °C

Global applicability domain: Inside

Local applicability domain index: 8.38e-01

Confidence level: 6.87e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isophorone

Measured: 215

Predicted: 207

[Image not found](#)

4-Methylcyclohex-3-en-1-one

Measured: 171

Predicted: 181

[Image not found](#)

2-Cyclohexen-1-one, 3,4,4-trimethyl-

Measured: 217

Predicted: 210