

1,1-dimethoxyhexan-2-one
6344-10-1 | DTXSID70287285

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: 193 °C

Global applicability domain: Inside

Local applicability domain index: 7.42e-01

Confidence level: 7.63e-01

Nearest Neighbors from the Training Set

Image not found

Isopropyl 4-oxovalerate

Measured: 209

Predicted: 194

Image not found

Ethyl isobutyrylacetate

Measured: 173

Predicted: 194

Image not found

Ethyl 2,2-dimethylacetoacetate

Measured: 182

Predicted: 190