

Dimethyl sulfoxide
67-68-5 | DTXSID2021735

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: 4.67e-01

Confidence level: 5.33e-01

Nearest Neighbors from the Training Set

Image not found

Dimethyl sulfoxide

Measured: 189

Predicted: 193

Image not found

beta-Propiolactone

Measured: 162

Predicted: 149

Image not found

Dimethyl sulfone

Measured: 238

Predicted: 218

Image not found

Dimethyl hydrogen phosphite

Measured: 171

Predicted: 168

Image not found

1,3-Dioxolan-2-one

Measured: 248

Predicted: 227