

Octaneperoxoic acid
33734-57-5 | DTXSID7074618

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: 238 °C

Global applicability domain: Inside

Local applicability domain index: 6.81e-01

Confidence level: 7.40e-01

Nearest Neighbors from the Training Set

Image not found

2-[2-(2-

Methoxyethoxy)ethoxy]ethanol

Measured: 249

Predicted: 243

Image not found

2-(2-Butoxyethoxy)ethanol

Measured: 231

Predicted: 228

Image not found

2-[2-(2-

Ethoxyethoxy)ethoxy]ethanol

Measured: 256

Predicted: 249

Image not found

Diethylene glycol monoisobutyl
ether

Measured: 217

Predicted: 219

Image not found

1-(2-Butoxyethoxy)-2-propanol

Measured: 230

Predicted: 226