

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 28.5 °C

Global applicability domain: Inside

Local applicability domain index: 5.01e-01

Confidence level: 4.67e-01

Nearest Neighbors from the Training Set

Image not found

Hydroperoxide, heptyl

Measured: 35.5

Predicted: 13.7

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tert-Butyl hydroperoxide

Measured: -8.00

Predicted: -23.0

Image not found

Hydroxyacetone

Measured: -17.0

Predicted: -6.56

Image not found

Octadecane-1-peroxol

Measured: 49.5

Predicted: 35.6

Image not found

Acetaldehyde, hydroxy-

Measured: 97.0

Predicted: 63.2