

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.48

Global applicability domain: Inside

Local applicability domain index: 5.90e-01

Confidence level: 7.73e-01

Nearest Neighbors from the Training Set

Image not found

2-Octanone

Measured: 2.37

Predicted: 2.42

Image not found

Geraniol

Measured: 3.56

Predicted: 3.38

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(2Z)-3,7-Dimethylocta-2,6-dien-1-ol

Measured: 3.56

Predicted: 3.38

Image not found

2-Heptanone

Measured: 1.98

Predicted: 1.88

Image not found

2,4-Dimethylpentan-3-one

Measured: 1.86

Predicted: 1.91

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1-Heptanol

Measured: 2.62

Predicted: 2.53