

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.55e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.43e-01

Confidence level: 5.65e-01

Nearest Neighbors from the Training Set

Image not found

Pentyl 2-hydroxypropanoate

Measured: 6.24e-02

Predicted: 1.34e-01

Image not found

Butyl lactate

Measured: 2.74e-01

Predicted: 2.78e-01

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Cumene hydroperoxide

Measured: 9.13e-02

Predicted: 4.16e-01

Image not found

Butyl 3-hydroxypropanoate

Measured: 5.13e-02

Predicted: 1.05e-01

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Octyl 2-hydroxypropanoate

Measured: 5.34e-02

Predicted: 3.96e-02