

Ethyl hydroperoxide
3031-74-1 | DTXSID70184402

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.21e-13 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.36e-01

Confidence level: 5.26e-01

Nearest Neighbors from the Training Set

Image not found

Epichlorohydrin

Measured: 4.40e-13

Predicted: 1.36e-12

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1,1-Dichloro-2-methoxyethane

Measured: 2.27e-12

Predicted: 1.81e-12

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1,1,1-Trichloroethane

Measured: 9.43e-15

Predicted: 3.29e-14

Image not found

1,1,2-Trichloroethane

Measured: 1.96e-13

Predicted: 6.60e-14

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2-Chloroethanol

Measured: 1.40e-12

Predicted: 2.40e-12