

Propaneperoxoic acid, 2-methyl-, 1,1-dimethylethyl ester
109-13-7 | DTXSID1059363

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.63 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.11e-01

Confidence level: 7.30e-01

Nearest Neighbors from the Training Set

Image not found

bis(2-Chloro-1-methylethyl) ether

Measured: 3.92

Predicted: 1.62

Image not found

Tetrahydrothiophene

Measured: 2.00

Predicted: 13.4

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Heptanoic acid

Measured: 2.34

Predicted: 6.20e-03

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Acetal

Measured: 10.8

Predicted: 33.8

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Nonanoic acid

Measured: 3.75e-01

Predicted: 1.91e-03