

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.37e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.73e-01

Confidence level: 7.08e-01

Nearest Neighbors from the Training Set

Image not found

2-Butoxyethyl acetate

Measured: 5.62e-02

Predicted: 6.06e-02

Image not found

Methyl 3-butoxypropanoate

Measured: 5.12e-02

Predicted: 5.88e-02

Image not found

Butyl 3-methoxypropionate

Measured: 6.12e-02

Predicted: 6.04e-02

Image not found

butyl 3-ethoxypropanoate

Measured: 2.30e-02

Predicted: 3.68e-02