

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.75

Global applicability domain: Inside

Local applicability domain index: 5.38e-01

Confidence level: 6.94e-01

Nearest Neighbors from the Training Set

Image not found

Linalool oxide

Measured: 2.43

Predicted: 3.03

Image not found

Heptyl acetate

Measured: 3.46

Predicted: 3.40

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2,4-Dimethylpentan-3-one

Measured: 1.86

Predicted: 1.91

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Methyl chrysanthemate (trans)

Measured: 3.76

Predicted: 3.56

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3-Methylbutyl acetate

Measured: 2.25

Predicted: 2.20