

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 7.12

Global applicability domain: Inside

Local applicability domain index: 4.97e-01

Confidence level: 5.95e-01

Nearest Neighbors from the Training Set

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O,O-Diethyl dithiophosphate

Measured: 5.01

Predicted: 5.43

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Thiram

Measured: 3.39

Predicted: 3.91

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Paraldehyde

Measured: 3.02

Predicted: 2.77

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2-
(Thiocyanomethylthio)benzothiazole

Measured: 209

Predicted: 13.0

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Dimethoate

Measured: 1.58

Predicted: 1.88