

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -58.7 °C

Global applicability domain: Inside

Local applicability domain index: 7.13e-01

Confidence level: 7.35e-01

Nearest Neighbors from the Training Set

Image not found

2-Butoxyethyl acetate

Measured: -63.0

Predicted: -54.2

Image not found

2-Ethoxyethyl acrylate

Measured: -47.0

Predicted: -54.7

Image not found

2-Ethoxyethyl acetate

Measured: -61.7

Predicted: -56.7

Image not found

2-Methoxyethyl acetate

Measured: -70.0

Predicted: -63.1

Image not found

Isobutyric anhydride

Measured: -53.5

Predicted: -56.2