

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 165 °C

Global applicability domain: Inside

Local applicability domain index: 7.14e-01

Confidence level: 7.47e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethane, 1,1,1-triethoxy-

Measured: 145

Predicted: 162

[Image not found](#)

Formic acid, heptyl ester

Measured: 178

Predicted: 171

[Image not found](#)

Methyl heptanoate

Measured: 174

Predicted: 169

[Image not found](#)

Butyl butyrate

Measured: 166

Predicted: 169

[Image not found](#)

Ethyl hexanoate

Measured: 167

Predicted: 170