

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.13e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.53e-01

Confidence level: 8.54e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Butyl butyrate

Measured: 1.06e-11

Predicted: 1.06e-11

[Image not found](#)

2-Ethoxyethyl isobutyrate

Measured: 1.35e-11

Predicted: 1.28e-11

[Image not found](#)

Pentyl acetate

Measured: 7.55e-12

Predicted: 6.38e-12

[Image not found](#)

Ethyl 3-ethoxypropionate

Measured: 2.29e-11

Predicted: 1.63e-11

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Butanoic acid, propyl ester

Measured: 7.41e-12

Predicted: 6.98e-12