

Sulfurous acid, bis(2-methylpropyl) ester
18748-27-1 | DTXSID30337997

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.93e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 5.52e-01

Nearest Neighbors from the Training Set

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Methyl butyrate

Measured: 1.18e-02

Predicted: 32.4

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Emylcamate

Measured: 7.24e-02

Predicted: 3.35e-01

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Furan, 2,3-dihydro-

Measured: 2.77e-01

Predicted: 200

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Hexamethylphosphoramide

Measured: 1.33e-02

Predicted: 7.54e-02

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Aspirin

Measured: 5.79e-01

Predicted: 1.03e-05