

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.65e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.19e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Dibutyl phosphite

Measured: 3.76e-02

Predicted: 4.20e-02

[Image not found](#)

Diisopropyl methylphosphonate

Measured: 8.88e-01

Predicted: 4.69e-01

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Phosphoric acid, diethyl propyl ester

Measured: 2.55

Predicted: 6.52e-01

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Triethyl phosphate

Measured: 2.74

Predicted: 1.41