

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.39

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 5.68e-01

Nearest Neighbors from the Training Set

Image not found

Tripropyl phosphate

Measured: 1.87

Predicted: 1.92

Image not found

Diisopropyl fluorophosphate

Measured: 1.17

Predicted: 1.28

Image not found

Tripropyl phosphite

Measured: 2.26

Predicted: 2.32

Image not found

Diisopropyl methylphosphonate

Measured: 1.03

Predicted: 1.40

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Phosphonic acid, bis(1-methylethyl) ester

Measured: 0.45

Predicted: 5.25e-01