

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.31

Global applicability domain: Inside

Local applicability domain index: 4.16e-01

Confidence level: 6.32e-01

Nearest Neighbors from the Training Set

Image not found

Triethyl phosphate

Measured: 1.29

Predicted: 1.38

Image not found

2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00

Predicted: 1.47

Image not found

Oxydisulfoton

Measured: 1.00

Predicted: 1.63

Image not found

Fenitrooxone

Measured: 2.75

Predicted: 1.68

Image not found

Triallyl phosphate

Measured: 1.20

Predicted: 1.41