

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 28.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 6.53e-01

Nearest Neighbors from the Training Set

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Aldicarb sulfoxide

Measured: 3.63

Predicted: 8.06

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Aldicarb

Measured: 31.6

Predicted: 38.0

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N-Cyclopropyl-N'-phenylurea

Measured: 55.0

Predicted: 74.0

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Propham

Measured: 67.6

Predicted: 83.2

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N-(3-chloro-4-methylphenyl)-N'-methylurea

Measured: 126

Predicted: 99.6