

Tris(2-chloroisopropyl)phosphate
13674-84-5 | DTXSID5026259

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: 2.15e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

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Tris(2-chloroisopropyl)phosphate

Measured: 3.66e-03

Predicted: 2.15e-03

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TDCPP

Measured: 1.62e-05

Predicted: 7.06e-05

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Tris(2-chloroethyl) phosphate

Measured: 2.45e-02

Predicted: 2.74e-02

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Naled

Measured: 5.25e-03

Predicted: 8.25e-03