

Tris(2-chloroethyl) phosphate
115-96-8 | DTXSID5021411

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: 2.74e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.53e-01

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

Image not found

Tris(2-chloroethyl) phosphate

Measured: 2.45e-02

Predicted: 2.74e-02

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Phosphoric acid, 2-chloroethenyl diethyl ester

Measured: 4.66e-02

Predicted: 4.25e-02

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Cyclophosphamide

Measured: 1.53e-01

Predicted: 8.08e-02

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Phosphonic acid, trichloromethyl-, diethyl ester

Measured: 1.76e-02

Predicted: 1.93e-02

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Naled

Measured: 5.25e-03

Predicted: 8.25e-03