

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

Model Performance

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: 2.81

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 5.04e-01

Nearest Neighbors from the Training Set

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Tris(2-chloroisopropyl)phosphate

Measured: 2.59

Predicted: 2.81

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Diallate

Measured: 4.49

Predicted: 4.18

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Pinacolyl
methylphosphonofluoridate

Measured: 1.78

Predicted: 2.07

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Tributyl phosphate

Measured: 4.00

Predicted: 3.60

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TDCPP

Measured: 3.65

Predicted: 3.71