

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.37×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.69×10^{-1}

Confidence level: 7.23×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Cycloate

Measured: 3.54×10^{-11}

Predicted: 2.98×10^{-11}

Image not found

Terbutylazine

Measured: 1.10×10^{-11}

Predicted: 1.23×10^{-11}

Image not found

EPTC

Measured: 3.18×10^{-11}

Predicted: 2.83×10^{-11}

Image not found

Simazine

Measured: 1.10×10^{-11}

Predicted: 1.22×10^{-11}

Image not found

Triethyl phosphate

Measured: 5.53×10^{-11}

Predicted: 4.26×10^{-11}