

4-(Chloromethyl)-2-ethoxy-1,3,2lambda⁵- dioxaphospholan-2-one

67554-11-4 | DTXSID50791173

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -58.9 °C

Global applicability domain: Inside

Local applicability domain index: 5.19e-01

Confidence level: 5.20e-01

Nearest Neighbors from the Training Set

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Dichlorvos

Measured: -60.0

Predicted: -45.2

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Tris(2-chloroisopropyl)phosphate

Measured: -40.0

Predicted: -39.4

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Tris(2-chloroethyl)phosphate

Measured: -35.0

Predicted: -30.9

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Diisopropyl fluorophosphate

Measured: -82.0

Predicted: -73.2

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Phosphonothioic acid, methyl-, O,o-diethyl ester

Measured: -84.4

Predicted: -62.3