

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 5.49e-02

Global applicability domain: Inside

Local applicability domain index: 3.35e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

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Dichlorvos

Measured: -0.300

Predicted: -0.189

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Tris(2-chloroethyl)
phosphate

Measured: 0.11

Predicted: 2.21e-01

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Triethyl phosphate

Measured: 0.11

Predicted: 1.40e-01

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Tris(2-
chloroisopropyl)phosphate

Measured: 0.9

Predicted: 8.22e-01

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Trimethyl phosphate

Measured: 0.15

Predicted: 1.75e-01