

Diethyl phosphorochloridate
814-49-3 | DTXSID4052556

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: 1.15

Global applicability domain: Inside

Local applicability domain index: 4.21e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

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Dichlorvos

Measured: 5.01e-01

Predicted: 6.47e-01

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Triethyl phosphate

Measured: 1.29

Predicted: 1.38

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00

Predicted: 1.47

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Paraldehyde

Measured: 3.02

Predicted: 2.77

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Trimethyl phosphate

Measured: 1.41

Predicted: 1.50