

Diisopropyl fluorophosphate
55-91-4 | DTXSID1040667

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: 2.25

Global applicability domain: Inside

Local applicability domain index: 4.26e-01

Confidence level: 8.18e-01

Nearest Neighbors from the Training Set

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o-Toluenesulfonamide

Measured: 2.57

Predicted: 2.00

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Benzenesulfonamide

Measured: 4.79

Predicted: 2.10

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Triallyl phosphate

Measured: 1.20

Predicted: 1.41

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Triethyl phosphate

Measured: 1.29

Predicted: 1.38

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Fenitrooxone

Measured: 2.75

Predicted: 1.68