

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.28e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.25e-01

Confidence level: 5.56e-01

Nearest Neighbors from the Training Set

Image not found

Aspirin

Measured: 5.79e-01

Predicted: 1.03e-05

Image not found

Furan, 2,3-dihydro-

Measured: 2.77e-01

Predicted: 200

Image not found

Hexamethylphosphoramide

Measured: 1.33e-02

Predicted: 7.54e-02

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Emylcamate

Measured: 7.24e-02

Predicted: 3.35e-01

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Cyclohexane, (1-methylethyl)-

Measured: 9.62e-01

Predicted: 4.19