

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -73.2 °C

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 7.72e-01

Nearest Neighbors from the Training Set

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Diisopropyl fluorophosphate

Measured: -82.0

Predicted: -73.2

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Trimethyl phosphate

Measured: -46.0

Predicted: -49.9

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Dimethyl hydrogen phosphite

Measured: -60.0

Predicted: -61.6

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Triethyl phosphate

Measured: -56.4

Predicted: -54.1

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Sarin

Measured: -57.0

Predicted: -59.2