

Ethyl perfluoropropionate
426-65-3 | DTXSID2059980

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.16e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.79e-01

Confidence level: 5.36e-01

Nearest Neighbors from the Training Set

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Ethyl 4,4,4-trifluoroacetoacetate

Measured: 4.35e-02

Predicted: 7.99e-02

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Diisopropyl fluorophosphate

Measured: 8.36e-02

Predicted: 8.23e-02

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Sarin

Measured: 7.14

Predicted: 1.65

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Pinacolyl
methylphosphonofluoridate

Measured: 1.15e-01

Predicted: 1.33e-01

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Mipafox

Measured: 4.39e-01

Predicted: 4.12e-01