

Perfluorododecanoic acid
307-55-1 | DTXSID8031861

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: 2.65e-01 mol/L

Global applicability domain: Outside

Local applicability domain index: 1.54e-01

Confidence level: 5.06e-01

Nearest Neighbors from the Training Set

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Fluopropanate-sodium

Measured: 1.31e-01

Predicted: 4.65e-01

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Acetic acid, trifluoro-

Measured: 8.77

Predicted: 4.36

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1,1,1-Trifluoro-2-propanol

Measured: 2.04

Predicted: 2.45

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3-Trifluoromethyl-4-nitrophenol

Measured: 2.41e-02

Predicted: 2.26e-01