

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.54

Global applicability domain: Outside

Local applicability domain index: 3.13e-01

Confidence level: 4.71e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Hexadecyl-2,4-dimethylpyridin-1-ium iodide

Measured: 3.90

Predicted: 4.51

[Image not found](#)

1-Hexadecyl-3,4-dimethylpyridin-1-ium iodide

Measured: 3.16

Predicted: 3.41

[Image not found](#)

1-Hexadecyl-3,5-dimethylpyridin-1-ium iodide

Measured: 3.35

Predicted: 3.41

[Image not found](#)

1-Octadecylpyridin-1-ium iodide

Measured: 3.68

Predicted: 4.50