

2,2,3,3,4,4,5,5,6,7,7,7-Dodecafluoro-6-(trifluoromethyl)heptanoic acid
15166-06-0 | DTXSID50562865

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 8.04e-13 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.38e-01

Confidence level: 5.80e-01

Nearest Neighbors from the Training Set

Image not found

1,1,2,3,3,3-Hexafluoro-1-propene

Measured: 2.20e-12

Predicted: 2.03e-12

Image not found

Acetic acid, trifluoro-

Measured: 1.20e-13

Predicted: 1.81e-13

Image not found

Trifluoro(trifluoromethoxy)ethylene

Measured: 3.58e-12

Predicted: 3.22e-12

Image not found

Acetic acid, trifluoro-, methyl ester

Measured: 5.20e-14

Predicted: 5.42e-14

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Chlorotrifluoroethylene

Measured: 7.00e-12

Predicted: 5.72e-12