

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
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.48e-01 mmHg

Global applicability domain: Outside

Local applicability domain index: 3.66e-01

Confidence level: 2.61e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Dichloro-4-(trifluoromethyl)benzene

Measured: 5.25e-01

Predicted: 2.42

Image not found

2-Butene, 1,1,1,2,3,4,4,4-octafluoro-

Measured: 1.33e-01

Predicted: 2800

Image not found

Benazolin

Measured: 4.28e-07

Predicted: 8.30e-09

Image not found

Bensulide

Measured: 2.48e-01

Predicted: 1.34e-06

Image not found

1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

Measured: 6.37

Predicted: 42.6