

1,1,2,2-Tetrafluoro-2-(1,1,2,2-tetrafluoroethoxy)ethane-1-sulfonyl fluoride
104729-49-9 | DTXSID40446988

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: 352 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.14e-01

Confidence level: 3.53e-01

Nearest Neighbors from the Training Set

Image not found

Mipafox

Measured: 41.2

Predicted: 1.79e-03

Image not found

1,1,1-Trifluoroethane

Measured: 4300

Predicted: 7650

Image not found

Ethyl propyl sulfide

Measured: 1.24e-01

Predicted: 17.9

Image not found

1-Dodecanamine

Measured: 48300

Predicted: 1.46e-02

Image not found

Ketene

Measured: 9410

Predicted: 1800