

Perfluoroheptanoic acid
375-85-9 | DTXSID1037303

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: 1.22e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.92e-01

Confidence level: 2.61e-01

Nearest Neighbors from the Training Set

[Image not found](#)

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

Measured: 1.33e-01

Predicted: 2800

[Image not found](#)

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

Measured: 5.25e-01

Predicted: 2.42

[Image not found](#)

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

Measured: 6.37

Predicted: 42.6

[Image not found](#)

Benazolin

Measured: 4.28e-07

Predicted: 8.30e-09

[Image not found](#)

Bensulide

Measured: 2.48e-01

Predicted: 1.34e-06