

1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-
2706-91-4 | DTXSID8062600

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 8.15e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.09e-01

Confidence level: 2.82e-01

Nearest Neighbors from the Training Set

Image not found

1-Propene, 3-propoxy-

Measured: 0.1

Predicted: 64.5

Image not found

Silane, chlorodimethylphenyl-

Measured: 2.91

Predicted: 1.01

Image not found

Fenamiphos

Measured: 3.00e-04

Predicted: 1.06e-06

Image not found

Bensulide

Measured: 2.48e-01

Predicted: 1.34e-06

Image not found

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

Measured: 1.33e-01

Predicted: 2800