

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 78.5 °C

Global applicability domain: Outside

Local applicability domain index: 2.63e-01

Confidence level: 6.33e-01

Nearest Neighbors from the Training Set

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Heptanoic acid,
2,2,3,3,4,4,5,5,6,6,7,7-
dodecafluoro-

Measured: 34.0

Predicted: 32.9

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Hexanedioic acid, 2,2,3,3,4,4,5,5-
octafluoro-

Measured: 134

Predicted: 123

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PFOA

Measured: 55.0

Predicted: 53.2

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Pentanedioic acid, hexafluoro-

Measured: 80.0

Predicted: 91.3

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Sulfluramid

Measured: 96.0

Predicted: 92.5