

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 223 °C

Global applicability domain: Outside

Local applicability domain index: 5.23e-01

Confidence level: 6.80e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Pentanesulfonic acid,
1,1,2,2,3,3,4,4,5,5,5-
undecafluoro-

Measured: 225

Predicted: 223

[Image not found](#)

PFHxS

Measured: 239

Predicted: 235

[Image not found](#)

1-Perfluorobutanesulfonic acid

Measured: 211

Predicted: 212

[Image not found](#)

Trifluoromethanesulfonic acid

Measured: 166

Predicted: 171

[Image not found](#)

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

Measured: 192

Predicted: 186