

Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-
1546-95-8 | DTXSID70165670

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: 186 °C

Global applicability domain: Outside

Local applicability domain index: 4.18e-01

Confidence level: 7.68e-01

Nearest Neighbors from the Training Set

Image not found

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

Measured: 192

Predicted: 186

Image not found

Perfluoroheptanoic acid

Measured: 177

Predicted: 176

Image not found

PFOA

Measured: 189

Predicted: 188

Image not found

Heptafluorobutyric acid

Measured: 121

Predicted: 120

Image not found

Pentafluoropropionic acid

Measured: 96.5

Predicted: 100