

Perfluoroheptanoic acid
375-85-9 | DTXSID1037303

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: 176 °C

Global applicability domain: Outside

Local applicability domain index: 5.32e-01

Confidence level: 7.68e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Perfluoroheptanoic acid

Measured: 177

Predicted: 176

[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](#)

PFOA

Measured: 189

Predicted: 188

[Image not found](#)

Heptafluorobutyric acid

Measured: 121

Predicted: 120

[Image not found](#)

Pentafluoropropionic acid

Measured: 96.5

Predicted: 100