

PFOA

335-67-1 | DTXSID8031865

Model Performance

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: 188 °C

Global applicability domain: Outside

Local applicability domain index: 4.18e-01

Confidence level: 6.38e-01

Nearest Neighbors from the Training Set

[Image not found](#)

PFOA

Measured: 189

Predicted: 188

[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](#)

Perfluorododecanoic acid

Measured: 249

Predicted: 244

[Image not found](#)

Heptafluorobutyric acid

Measured: 121

Predicted: 120