

# PFOA

335-67-1 | DTXSID8031865

## Model Performance

### Weighted KNN model

#### 5-fold CV (75%)

#### Training (75%)

#### Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** 53.2 °C

**Global applicability domain:** Outside

**Local applicability domain index:** 4.51e-01

**Confidence level:** 6.20e-01

## Nearest Neighbors from the Training Set

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PFOA

**Measured:** 55.0

**Predicted:** 53.2

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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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1-Nonanol,  
2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-  
hexadecafluoro-

**Measured:** 56.0

**Predicted:** 54.2

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Perfluorododecanoic acid

**Measured:** 108

**Predicted:** 103

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Heptafluorobutyric acid

**Measured:** -17.5

**Predicted:** -14.1