

# PFOA

335-67-1 | DTXSID8031865

## Model Performance

### Weighted KNN model

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

#### Training (75%)

#### Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** 3.74

**Global applicability domain:** Inside

**Local applicability domain index:** 3.92e-01

**Confidence level:** 3.95e-01

## Nearest Neighbors from the Training Set

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1,1,2,2-Tetrahydroperfluoro-  
1-decanol

**Measured:** 5.58

**Predicted:** 5.05

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3,3,4,4,5,5,6,6,7,7,8,8,8-  
Tridecafluorooctan-1-ol

**Measured:** 4.54

**Predicted:** 4.45

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Perflenapent

**Measured:** 4.40

**Predicted:** 4.23

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1-Dodecyl-2,4-  
dimethylpyridin-1-ium iodide

**Measured:** 1.41

**Predicted:** N/A

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1-Dodecyl-2-methylpyridin-  
1-ium iodide

**Measured:** 1.32

**Predicted:** N/A