

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
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** 35.5 °C

**Global applicability domain:** Outside

**Local applicability domain index:** 4.26e-01

**Confidence level:** 8.39e-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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Heptafluorobutyric acid

**Measured:** -17.5

**Predicted:** -14.1

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1,1,1,3,3,3-Hexafluoro-2-  
propanol

**Measured:** -4.00

**Predicted:** -8.02