

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
0.84	0.55	0.85	0.53	0.83	0.64

## Model Results

**Predicted value:** 4.99

**Global applicability domain:** Outside

**Local applicability domain index:** 2.00e-01

**Confidence level:** 8.01e-01

## Nearest Neighbors from the Training Set

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4-Hydroxy-1-naphthalenesulfonic acid monosodium salt

**Measured:** 12.9

**Predicted:** 6.33

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2-Amino-1-naphthalenesulfonic acid

**Measured:** 6.03

**Predicted:** 6.40

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Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

**Measured:** 3.02

**Predicted:** 5.14

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Sodium 3-nitrobenzenesulfonate

**Measured:** 5.01

**Predicted:** 5.24

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

**Measured:** 2.51

**Predicted:** 2.40