

1-Hexanol, 3,3,4,4,5,5,6,6,6-nonafluoro-  
2043-47-2 | DTXSID1062122

## 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:** 4.02 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 3.66e-01

**Confidence level:** 8.17e-01

## Nearest Neighbors from the Training Set

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

**Measured:** -4.00

**Predicted:** -8.02

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Heptafluorobutyric acid

**Measured:** -17.5

**Predicted:** -14.1

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1-Propanol, 2,2,3,3-tetrafluoro-

**Measured:** -15.0

**Predicted:** -15.0

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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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Pentafluorophenol

**Measured:** 32.8

**Predicted:** 37.3