

Hexanedioic acid, 2,2,3,3,4,4,5,5-octafluoro-  
336-08-3 | DTXSID4059833

## 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:** 123 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 4.21e-01

**Confidence level:** 6.29e-01

## Nearest Neighbors from the Training Set

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Hexanedioic acid, 2,2,3,3,4,4,5,5-octafluoro-

**Measured:** 134

**Predicted:** 123

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Pentanedioic acid, hexafluoro-

**Measured:** 80.0

**Predicted:** 91.3

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Butanedioic acid, 2,2,3,3-tetrafluoro-

**Measured:** 119

**Predicted:** 116

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1,5-Pentanediol, 2,2,3,3,4,4-hexafluoro-

**Measured:** 79.5

**Predicted:** 76.4

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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