

Pentanedioic acid, hexafluoro-  
376-73-8 | DTXSID8059926

## 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:** 3.78

**Global applicability domain:** Outside

**Local applicability domain index:** 2.01e-01

**Confidence level:** 7.92e-01

## Nearest Neighbors from the Training Set

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7-Amino-4-hydroxynaphthalene-  
2-sulfonic acid

**Measured:** 2.40

**Predicted:** 4.77

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6-Amino-4-hydroxynaphthalene-  
2-sulfonic acid

**Measured:** 4.07

**Predicted:** 4.77

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2-Amino-5-  
methylbenzenesulfonic acid

**Measured:** 3.98

**Predicted:** 6.29

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4-Hydroxy-1-naphthalenesulfonic  
acid monosodium salt

**Measured:** 12.9

**Predicted:** 6.33