

Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-
1546-95-8 | DTXSID70165670

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: 5.91

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 8.04e-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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Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

Measured: 3.02

Predicted: 5.14

Image not found

Sodium 3-nitrobenzenesulfonate

Measured: 5.01

Predicted: 5.24

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2-Amino-1-naphthalenesulfonic acid

Measured: 6.03

Predicted: 6.40

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4-Amino-1-naphthalenesulfonic acid sodium salt

Measured: 6.03

Predicted: 5.38