

1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-
2706-91-4 | DTXSID8062600

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.87e-01 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.23e-01

Confidence level: 5.25e-01

Nearest Neighbors from the Training Set

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4-Methylbenzenesulfonic acid

Measured: 3.60

Predicted: 2.37

Image not found

Methylarsonic acid

Measured: 1.83

Predicted: N/A

Image not found

Monosodium methanearsonate

Measured: 3.58

Predicted: N/A

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Fluopropanate-sodium

Measured: 1.31e-01

Predicted: 4.65e-01