

1,1,2,3,3,3-Hexafluoro-2-(trifluoromethyl)propanesulphonic acid
93762-09-5 | DTXSID90239569

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 213 °C

Global applicability domain: Outside

Local applicability domain index: 3.60e-01

Confidence level: 6.80e-01

Nearest Neighbors from the Training Set

Image not found

1-Perfluorobutanesulfonic acid

Measured: 211

Predicted: 212

Image not found

1-Pentanesulfonic acid,
1,1,2,2,3,3,4,4,5,5-
undecafluoro-

Measured: 225

Predicted: 223

Image not found

PFHxS

Measured: 239

Predicted: 235

Image not found

Trifluoromethanesulfonic acid

Measured: 166

Predicted: 171

Image not found

Heptanoic acid,
2,2,3,3,4,4,5,5,6,6,7,7-
dodecafluoro-

Measured: 192

Predicted: 186