

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.34e-15 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.78e-01

Nearest Neighbors from the Training Set

Image not found

2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane

Measured: 7.50e-14

Predicted: 3.74e-14

Image not found

Perfluorotriethylamine

Measured: 6.00e-16

Predicted: 6.45e-16

Image not found

Perfluorotributylamine

Measured: 6.00e-17

Predicted: 1.14e-16

Image not found

Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-

Measured: 7.20e-15

Predicted: 1.32e-14