

1-Perfluorobutanesulfonic acid

375-73-5 | DTXSID5030030

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

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: -14.7 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.56e-01

Confidence level: 4.78e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Perfluorotriethylamine

Measured: -15.2

Predicted: -15.2

[Image not found](#)

Perfluorotributylamine

Measured: -16.2

Predicted: -15.9

[Image not found](#)

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

Measured: -14.1

Predicted: -13.9

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2-(Difluoromethoxy)-

1,1,1,3,3,3-

hexafluoropropane

Measured: -13.1

Predicted: -13.4