

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%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.00e-01

Global applicability domain: Outside

Local applicability domain index: 2.48e-01

Confidence level: 8.21e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Hydroxy-1-naphthalenesulfonic acid monosodium salt

Measured: 1.11

Predicted: 8.08e-01

[Image not found](#)

2-Amino-1-naphthalenesulfonic acid

Measured: 0.78

Predicted: 8.06e-01

[Image not found](#)

2-Amino-5-methylbenzenesulfonic acid

Measured: 0.6

Predicted: 7.98e-01

[Image not found](#)

4-Amino-1-naphthalenesulfonic acid sodium salt

Measured: 0.78

Predicted: 7.49e-01

[Image not found](#)

Sodium 3-nitrobenzenesulfonate

Measured: 0.7

Predicted: 7.21e-01