

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 70.6 °C

Global applicability domain: Inside

Local applicability domain index: 2.82e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

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Hexanedioic acid,
2,2,3,3,4,4,5,5-octafluoro-

Measured: 134

Predicted: 123

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

Measured: 34.0

Predicted: 32.9

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Pentanedioic acid,
hexafluoro-

Measured: 80.0

Predicted: 91.3

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Heptafluorobutyric acid

Measured: -17.5

Predicted: -14.1

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Butanedioic acid, 2,2,3,3-
tetrafluoro-

Measured: 119

Predicted: 116