

1-Butanol, 2,2,3,3,4,4,4-heptafluoro-
375-01-9 | DTXSID4059914

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: -16.4 °C

Global applicability domain: Inside

Local applicability domain index: 4.41e-01

Confidence level: 7.60e-01

Nearest Neighbors from the Training Set

Image not found

1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: -4.00

Predicted: -8.02

Image not found

Heptafluorobutyric acid

Measured: -17.5

Predicted: -14.1

Image not found

1-Propanol, 2,2,3,3-tetrafluoro-

Measured: -15.0

Predicted: -15.0

Image not found

2,2,2-Trifluoroethanol

Measured: -43.5

Predicted: -35.9

Image not found

Acetic acid, trifluoro-

Measured: -15.2

Predicted: -15.5