

1-Nonanol, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-hexadecafluoro-
376-18-1 | DTXSID3059923

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 148 °C

Global applicability domain: Outside

Local applicability domain index: 2.70e-01

Confidence level: 6.36e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1-Octanol,
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-
pentadecafluoro-

Measured: 161

Predicted: 156

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Methyl perfluorooctanoate

Measured: 158

Predicted: 151