

1-Hexanol, 3,3,4,4,5,5,6,6-nonafluoro-
2043-47-2 | DTXSID1062122

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: 101 °C

Global applicability domain: Inside

Local applicability domain index: 3.76e-01

Confidence level: 5.61e-01

Nearest Neighbors from the Training Set

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1-Pentanol, 2,2,3,3,4,4,5,5-octafluoro-

Measured: 141

Predicted: 129

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1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

Measured: 95.0

Predicted: 96.9

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2-Propanol, 1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)-

Measured: 45.0

Predicted: 55.1

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

Measured: 59.0

Predicted: 70.9