

1-Octanol
111-87-5 | DTXSID7021940

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: -22.1 °C

Global applicability domain: Inside

Local applicability domain index: 9.27e-01

Confidence level: 4.42e-01

Nearest Neighbors from the Training Set

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1-Octanol

Measured: -15.5

Predicted: -22.1

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6-Methyl-1-heptanol

Measured: -106

Predicted: -30.6

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1-Nonanol

Measured: -5.00

Predicted: -7.41

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1-Heptanol

Measured: -34.0

Predicted: -47.4

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7-Methyl-1-octanol

Measured: 64.5

Predicted: -0.841