

1-Pentanol
71-41-0 | DTXSID6021741

Model Performance

Model	Data
-------	------

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: -87.1 °C

Global applicability domain: Inside

Local applicability domain index: 8.62e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found

1-Pentanol

Measured: -78.9

Predicted: -87.1

Image not found

Isopentyl alcohol

Measured: -117

Predicted: -96.2

Image not found

1-Hexanol

Measured: -44.6

Predicted: -61.5

Image not found

2-Methyl-1-propanol

Measured: -108

Predicted: -103

Image not found

1-Butanol

Measured: -89.8

Predicted: -95.0