

2,2,4-Trimethyl-1,3-pentanediol
144-19-4 | DTXSID8027113

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: 40.7 °C

Global applicability domain: Inside

Local applicability domain index: 7.32e-01

Confidence level: 4.95e-01

Nearest Neighbors from the Training Set

Image not found

2,2,4-Trimethyl-1,3-pentanediol

Measured: 51.5

Predicted: 40.7

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2-Ethyl-1,3-hexanediol

Measured: -40.0

Predicted: -7.80

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2,5-Dimethylhexane-2,5-diol

Measured: 92.0

Predicted: 63.2

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2,3-Butanediol, 2,3-dimethyl-

Measured: 43.0

Predicted: 40.0

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2-Butyl-2-ethyl-1,3-propanediol

Measured: 43.8

Predicted: 25.0