

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 229 °C

Global applicability domain: Inside

Local applicability domain index: 7.84e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

Image not found

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

Measured: 232

Predicted: 229

Image not found

2,5-Dimethylhexane-2,5-diol

Measured: 214

Predicted: 226

Image not found

2-Ethyl-1,3-hexanediol

Measured: 244

Predicted: 239

Image not found

Prenderol

Measured: 241

Predicted: 240

Image not found

1,3-Propanediol, 2-methyl-2-propyl-

Measured: 234

Predicted: 239