

1,3-Naphthalenediol
132-86-5 | DTXSID8059631

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: 290 °C

Global applicability domain: Inside

Local applicability domain index: 3.51e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

Image not found

(1,1'-Biphenyl)-2,2'-diol

Measured: 320

Predicted: 315

Image not found

2,3-Dihydroxybenzaldehyde

Measured: 235

Predicted: 253

Image not found

tert-Butylhydroquinone

Measured: 273

Predicted: 277

Image not found

4-tert-Butylcatechol

Measured: 285

Predicted: 277

Image not found

4-Hexylresorcinol

Measured: 334

Predicted: 302