

phenol, 4,4'-butylidenebis-
4731-84-4 | DTXSID20280701

Model Performance

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

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: 347 °C

Global applicability domain: Inside

Local applicability domain index: 2.95e-01

Confidence level: 5.61e-01

Nearest Neighbors from the Training Set

Image not found

2,2'-Dihydroxybenzophenone

Measured: 333

Predicted: 318

Image not found

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

Measured: 320

Predicted: 315

Image not found

4-Hexylresorcinol

Measured: 334

Predicted: 302

Image not found

Alizarin

Measured: 430

Predicted: 399

Image not found

Benzoin

Measured: 344

Predicted: 319

Image not found

Benzoin

Measured: 344

Predicted: 319