

Phenol, 2-[1-(4-hydroxyphenyl)-1-methylethyl]-
837-08-1 | DTXSID7042275

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: 164 °C

Global applicability domain: Inside

Local applicability domain index: 7.23e-01

Confidence level: 5.07e-01

Nearest Neighbors from the Training Set

Image not found

3,3'-Dimethylbisphenol A

Measured: 139

Predicted: 157

Image not found

[1,1'-Biphenyl]-4,4'-diol, 3,3',5,5'-
tetramethyl-

Measured: 222

Predicted: 188

Image not found

Menadiol

Measured: 169

Predicted: 138

Image not found

1,4-Benzenediol, 2-
(phenylmethyl)-

Measured: 106

Predicted: 117

Image not found

meso-Hexestrol

Measured: 187

Predicted: 157