

Pyrogallol
87-66-1 | DTXSID6025983

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: 292 °C

Global applicability domain: Outside

Local applicability domain index: 2.74e-01

Confidence level: 6.02e-01

Nearest Neighbors from the Training Set

Image not found

Pyrogallol

Measured: 309

Predicted: 292

Image not found

2-(Hydroxymethyl)-2-methyl-1,3-propanediol

Measured: 283

Predicted: 289

Image not found

1,2,4-Butanetriol

Measured: 312

Predicted: 300

Image not found

1,2-Benzenediol, 3-methyl-

Measured: 241

Predicted: 257

Image not found

4-Methylcatechol

Measured: 251

Predicted: 257