

4-Hexylresorcinol
136-77-6 | DTXSID1020699

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: 302 °C

Global applicability domain: Inside

Local applicability domain index: 4.88e-01

Confidence level: 6.65e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Hexylresorcinol

Measured: 334

Predicted: 302

[Image not found](#)

tert-Butylhydroquinone

Measured: 273

Predicted: 277

[Image not found](#)

4-tert-Butylcatechol

Measured: 285

Predicted: 277

[Image not found](#)

4-Isopropylcatechol

Measured: 271

Predicted: 277