

tert-Butylhydroquinone
1948-33-0 | DTXSID6020220

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.46e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.31e-01

Confidence level: 6.50e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 1.45e-01

Predicted: 2.34e-01

[Image not found](#)

Terpin

Measured: 2.06e-02

Predicted: 3.89e-02

[Image not found](#)

Terpin

Measured: 2.06e-02

Predicted: 3.89e-02

[Image not found](#)

Tribromoacetic acid

Measured: 6.74e-01

Predicted: 5.34e-01