

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.05e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.54e-01

Confidence level: 4.35e-01

Nearest Neighbors from the Training Set

Image not found

3-Phenyl-1-propanol

Measured: 2.21e-03

Predicted: 5.06e-02

Image not found

Endothal

Measured: 1.66e-03

Predicted: 9.06e-10

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4-Methoxyaniline

Measured: 3.08e-04

Predicted: 3.72e-02

Image not found

N,N-Dimethylformamide

Measured: 8.20e-05

Predicted: 5.14

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4-Isopropylphenol

Measured: 1.92e-07

Predicted: 3.08e-02