

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 91.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.17e-01

Confidence level: 6.01e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Acetyl-m-toluidine

Measured: 28.2

Predicted: 42.1

[Image not found](#)

1-Naphthylamine

Measured: 3240

Predicted: 1020

[Image not found](#)

Isophorone

Measured: 25.1

Predicted: 103

[Image not found](#)

Acetamide, N-(2-chlorophenyl)-

Measured: 38.0

Predicted: 49.2

[Image not found](#)

Acetamide, N-(3-chlorophenyl)-

Measured: 72.4

Predicted: 55.5