

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.15e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.31e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Naphthoquinone

Measured: 3.10e-12

Predicted: 3.16e-11

Image not found

2-Methyl-p-benzoquinone

Measured: 2.35e-11

Predicted: 2.15e-11

Image not found

(2E)-2-Hexenal

Measured: 4.40e-11

Predicted: 4.31e-11

Image not found

(2E)-3-Phenylprop-2-enal

Measured: 4.80e-11

Predicted: 5.31e-11