

phenol, 4,4'-butylidenebis-
4731-84-4 | DTXSID20280701

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 33.3

Global applicability domain: Inside

Local applicability domain index: 4.46e-01

Confidence level: 5.76e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Disulfoton

Measured: 219

Predicted: 151

[Image not found](#)

Oxydisulfoton

Measured: 1.00

Predicted: 1.63

[Image not found](#)

Parathion

Measured: 97.7

Predicted: 22.3

[Image not found](#)

Isoamyl ether

Measured: 170

Predicted: 137

[Image not found](#)

Menthol

Measured: 10.8

Predicted: 23.5

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(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5