

Guanidine, N,N"-((iminodi-8,1-octanediy))bis-
13516-27-3 | DTXSID7042015

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.66 days

Global applicability domain: Inside

Local applicability domain index: 4.24e-01

Confidence level: 8.40e-01

Nearest Neighbors from the Training Set

Image not found

Propylbenzene

Measured: 24.3

Predicted: 4.02

Image not found

4-Ethyltoluene

Measured: 24.3

Predicted: 3.95

Image not found

1,2-Dimethyl-4-ethylbenzene

Measured: 40.7

Predicted: 4.08

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 24.3

Predicted: 3.89

Image not found

1,3-Dimethyl-5-ethylbenzene

Measured: 4.93

Predicted: 3.64