

Tetrachlorophthalic acid
632-58-6 | DTXSID6060896

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 14.8 days

Global applicability domain: Outside

Local applicability domain index: 2.39e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

Image not found

9-Ethyl-9H-fluorene

Measured: 2330

Predicted: N/A

Image not found

5-Methylindan

Measured: 4.93

Predicted: 2.25

Image not found

2-Methylphenanthrene

Measured: 1370

Predicted: 25.0

Image not found

4-Phenyltoluene

Measured: 4340

Predicted: 25.1

Image not found

2-Methylnaphthalene

Measured: 436

Predicted: 15.3