

Phenanthrene, trimethyl-
30232-26-9 | DTXSID90184328

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: 75.6 days

Global applicability domain: Inside

Local applicability domain index: 5.96e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

Image not found

Phenanthrene, trimethyl-

Measured: 26200

Predicted: 75.6

Image not found

1-Methyl phenanthrene

Measured: 1370

Predicted: 36.9

Image not found

11H-Benzo[a]fluorene

Measured: 88900

Predicted: 121

Image not found

9-Methylanthracene

Measured: 364000

Predicted: 144

Image not found

2-Methylphenanthrene

Measured: 1370

Predicted: 25.0