

Heptachlor epoxide
1024-57-3 | DTXSID1024126

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: 110 days

Global applicability domain: Outside

Local applicability domain index: 1.67e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

Image not found

Octahydro-exo-4,7-methano-1H-indene

Measured: 8090000

Predicted: 636

Image not found

Squalane

Measured: 5460

Predicted: 49.4

Image not found

Phenanthrene, trimethyl-

Measured: 26200

Predicted: 75.6

Image not found

11H-Benzo[a]fluorene

Measured: 88900

Predicted: 121

Image not found

9-Ethyl-9H-fluorene

Measured: 2330

Predicted: N/A