

Hexachlorophene
70-30-4 | DTXSID6020690

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 102000 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.89e-01

Confidence level: 6.02e-01

Nearest Neighbors from the Training Set

Image not found

Dicofol

Measured: 5010

Predicted: 8300

Image not found

Leptophos

Measured: 31600

Predicted: 6220

Image not found

2,2',3,4,5,5',6-
Heptachlorobiphenyl

Measured: 891000

Predicted: 1020000

Image not found

2,2',3,3',4,4'-Hexachlorobiphenyl

Measured: 457000

Predicted: 631000

Image not found

p,p'-DDT

Measured: 204000

Predicted: 105000