

Chlorothalonil
1897-45-6 | DTXSID0020319

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 231 °C

Global applicability domain: Inside

Local applicability domain index: 4.12e-01

Confidence level: 4.56e-01

Nearest Neighbors from the Training Set

Image not found

Chlorothalonil

Measured: 250

Predicted: 231

Image not found

1,2-Benzenedicarbonitrile

Measured: 140

Predicted: 168

Image not found

1,3-Benzenedicarbonitrile

Measured: 162

Predicted: 168

Image not found

1,4-Benzenedicarbonitrile

Measured: 224

Predicted: 169

Image not found

(2-Chlorobenzylidene)propanedinitrile

Measured: 95.5

Predicted: 90.2