

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
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 5.39e-13 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:** 2.41e-01

**Confidence level:** 6.45e-01

## Nearest Neighbors from the Training Set

Image not found

Dimethyl sulfate

**Measured:** 5.00e-13

**Predicted:** 4.96e-13

Image not found

Diethyl sulfate

**Measured:** 1.80e-12

**Predicted:** 1.55e-12

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Propylene dinitrate

**Measured:** 3.20e-13

**Predicted:** 3.59e-13

Image not found

2-Nitrophenol

**Measured:** 9.00e-13

**Predicted:** 1.33e-11

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Nitrobenzene

**Measured:** 1.40e-13

**Predicted:** 1.97e-11