

Chlorbromuron
13360-45-7 | DTXSID6040290

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.51e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.27e-01

Confidence level: 4.67e-01

Nearest Neighbors from the Training Set

Image not found

1,2,2,3-Tetrachloropropane

Measured: 3.97e-07

Predicted: 2.35

Image not found

4-Hydroxy-3-nitrobenzaldehyde

Measured: 3.00e-06

Predicted: 1.26e-03

Image not found

Methyltris(trimethylsiloxy)silane

Measured: 3.23e-05

Predicted: 8.44e-02

Image not found

Aldrin

Measured: 1.43e-06

Predicted: 7.07e-05

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2,3,7,8-Tetrachlorodibenzo-p-dioxin

Measured: 1.50e-04

Predicted: 5.44e-09