

Tetrachloroethylene

127-18-4 | DTXSID2021319

Model Performance

Model

Data

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: -12.6 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.63e-01

Confidence level: 6.35e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Tetrachloroethylene

Measured: -12.8

Predicted: -12.6

[Image not found](#)

Trichloroethylene

Measured: -11.6

Predicted: -11.7

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Chloral

Measured: -11.8

Predicted: -11.8

[Image not found](#)

Oxazole

Measured: -11.0

Predicted: -10.5