

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 |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: -13.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 3.10e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Tetrachloroethylene

Measured: -22.3

Predicted: -13.3

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Hexachloropropene

Measured: -72.9

Predicted: -34.7

[Image not found](#)

Hexachloroethane

Measured: 187

Predicted: 118

[Image not found](#)

Dichloroacetylene

Measured: -66.0

Predicted: -65.0

[Image not found](#)

Hexachloro-1,3-butadiene

Measured: -21.0

Predicted: -20.7