

Chloromethane
74-87-3 | DTXSID0021541

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 |

Model Results

Predicted value: 12.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.86e-01

Confidence level: 8.36e-01

Nearest Neighbors from the Training Set

Image not found

Thioacetamide

Measured: 6.03

Predicted: 6.43

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Methyl isothiocyanate

Measured: 9.33

Predicted: 7.63

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1,1-Dichloroethane

Measured: 30.2

Predicted: 34.4

Image not found

1,2-Dichloroethane

Measured: 33.1

Predicted: 32.5

Image not found

Ethyleneimine

Measured: 6.03

Predicted: 4.17