

Chloropicrin
76-06-2 | DTXSID0020315

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.93 | 22.5 | 0.93 | 22.1 | 0.93 | 22.1 |

Model Results

Predicted value: 127 °C

Global applicability domain: Inside

Local applicability domain index: 7.46e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

Image not found

Chloropicrin

Measured: 112

Predicted: 127

Image not found

1,1-Dichloro-1-nitroethane

Measured: 124

Predicted: 136

Image not found

2-Bromo-2-nitropropane

Measured: 153

Predicted: 145

Image not found

Propane, 1,1-dichloro-1-nitro-

Measured: 145

Predicted: 143

Image not found

1-Chloro-2-nitropropane

Measured: 173

Predicted: 162