

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
26946-56-5 | DTXSID10447169

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 2.15

Global applicability domain: Inside

Local applicability domain index: 6.10e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

Image not found

Isophorone

Measured: 1.70

Predicted: 2.28

Image not found

L-Verbenone

Measured: 2.23

Predicted: 2.39

Image not found

6,6-Dimethylbicyclo[3.1.1]heptane-2-carbaldehyde

Measured: 2.98

Predicted: 2.78

Image not found

5,5-Dimethylhexane-2,4-dione

Measured: 1.67

Predicted: 1.83