

Ethane
74-84-0 | DTXSID6026377

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 13000 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.04e-01

Confidence level: 6.50e-01

Nearest Neighbors from the Training Set

Image not found

Methyl bromide

Measured: 31500

Predicted: 665

Image not found

Diethyl sulfide

Measured: 6840

Predicted: 45.4

Image not found

1,3-Butadiyne

Measured: 2010

Predicted: 1030

Image not found

Bromochloromethane

Measured: 7150

Predicted: 198

Image not found

Vinyl chloride

Measured: 19800

Predicted: 1530