

Acetic acid, trifluoro-, methyl ester
431-47-0 | DTXSID2059988

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: -50.1 °C

Global applicability domain: Inside

Local applicability domain index: 4.61e-01

Confidence level: 4.42e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl perfluoropropionate

Measured: 75.5

Predicted: 43.9

[Image not found](#)

1,2-Dichloro-1,1,2-trifluoroethane

Measured: -78.0

Predicted: -95.4

[Image not found](#)

1,2-Dichloro-3,3,3-trifluoroprop-1-ene

Measured: -109

Predicted: -109

[Image not found](#)

2,2-Dichloro-1,1,1-trifluoroethane

Measured: -107

Predicted: -104