

Butanedioic acid, 2,2,3,3-tetrafluoro-
377-38-8 | DTXSID8059928

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: 318 °C

Global applicability domain: Outside

Local applicability domain index: 2.41e-01

Confidence level: 5.44e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Pentanedioic acid

Measured: 303

Predicted: 310

[Image not found](#)

Hexanedioic acid

Measured: 338

Predicted: 330

[Image not found](#)

Heptanedioic acid

Measured: 342

Predicted: 332

[Image not found](#)

Octanedioic acid

Measured: 346

Predicted: 332

[Image not found](#)

3-Ethyl-3-methylglutaric acid

Measured: 261

Predicted: 286