

1,1,1,3,3-Pentafluoro-3-(1,2,2,2-tetrafluoroethoxy)propan-2-one
88457-11-8 | DTXSID00748238

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: 52.8 °C

Global applicability domain: Inside

Local applicability domain index: 4.72e-01

Confidence level: 8.33e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Cyclohexene, 1,2,3,3,4,4,5,5,6,6-decafluoro-

Measured: 52.0

Predicted: 52.8

[Image not found](#)

Butanoyl chloride, heptafluoro-

Measured: 38.5

Predicted: 40.8

[Image not found](#)

Cyclohexane, undecafluoro-

Measured: 62.0

Predicted: 58.2