

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol
647-42-7 | DTXSID5044572

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: 31.3 °C

Global applicability domain: Outside

Local applicability domain index: 3.53e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

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1-Nonanol,
2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-
hexadecafluoro-

Measured: 56.0

Predicted: 54.2

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Heptanoic acid,
2,2,3,3,4,4,5,5,6,6,7,7-
dodecafluoro-

Measured: 34.0

Predicted: 32.9

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PFOA

Measured: 55.0

Predicted: 53.2

Image not found

Heptafluorobutyric acid

Measured: -17.5

Predicted: -14.1

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1,1,1,3,3,3-Hexafluoro-2-
propanol

Measured: -4.00

Predicted: -8.02