

Tetradecane
629-59-4 | DTXSID1027267

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: 3.94 °C

Global applicability domain: Inside

Local applicability domain index: 9.90e-01

Confidence level: 9.44e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Tetradecane

Measured: 5.80

Predicted: 3.94

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Pentadecane

Measured: 9.90

Predicted: 10.3

[Image not found](#)

Tridecane

Measured: -5.30

Predicted: -4.65

[Image not found](#)

Hexadecane

Measured: 18.1

Predicted: 16.9

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Dodecane

Measured: -9.60

Predicted: -12.6