

2,3,4-Trimethylpentane
565-75-3 | DTXSID6060343

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 25.3 mmHg

Global applicability domain: Inside

Local applicability domain index: 9.15e-01

Confidence level: 8.36e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,1-Dichloro-1-nitroethane

Measured: 20.9

Predicted: 11.0

[Image not found](#)

3,3-Dimethyl-1-butene

Measured: 27.0

Predicted: 280

[Image not found](#)

Endosulfan sulfate

Measured: 23.0

Predicted: 2.61e-07

[Image not found](#)

1-Propene, 3-ethoxy-

Measured: 28.6

Predicted: 160