

Pentanedioic acid, 3,3-dimethyl-
4839-46-7 | DTXSID9063617

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.81 | 0.55 | 0.81 | 0.54 | 0.71 | 0.61 |

Model Results

Predicted value: 28.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.57e-01

Confidence level: 5.74e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2

[Image not found](#)

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

[Image not found](#)

1-Methoxy-2-propyl acetate

Measured: 2.29

Predicted: 7.33

[Image not found](#)

Urea, (m-fluorophenyl)-

Measured: 58.9

Predicted: 59.1

[Image not found](#)

Metaldehyde acetaldehyde
tetramer

Measured: 240

Predicted: 148