

2,2-Dimethylpentanedioic acid
681-57-2 | DTXSID6021585

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: 90.5 °C

Global applicability domain: Inside

Local applicability domain index: 8.48e-01

Confidence level: 6.42e-01

Nearest Neighbors from the Training Set

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2,2-Dimethylpentanedioic acid

Measured: 84.0

Predicted: 90.5

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2-METHYLHEXANEDIOIC ACID

Measured: 64.0

Predicted: 90.6

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Pentanedioic acid, 3,3-dimethyl-

Measured: 104

Predicted: 96.7

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3-Ethyl-3-methylglutaric acid

Measured: 87.0

Predicted: 88.7

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Octanedioic acid

Measured: 144

Predicted: 115