

2,2,8-Trimethyl-7-prop-2-ynoxchromene
94244-29-8 | DTXSID10241225

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: 66.9 °C

Global applicability domain: Inside

Local applicability domain index: 4.33e-01

Confidence level: 5.93e-01

Nearest Neighbors from the Training Set

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Ethanol, 2-(1-naphthalenyloxy)-

Measured: 45.0

Predicted: 69.9

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4-(Benzyloxy)phenol

Measured: 122

Predicted: 95.1

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4-Phenoxyphenol

Measured: 84.0

Predicted: 87.2

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4-(4-Methoxyphenyl)butan-1-ol

Measured: 3.50

Predicted: 31.5