

Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, methyl ester  
145348-22-7 | DTXSID60162991

### 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:** 107 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 8.48e-01

**Confidence level:** 7.25e-01

## Nearest Neighbors from the Training Set

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Cyclopropanecarboxylic acid, 1-  
((4-chlorophenyl)sulfonyl)-,  
methyl ester

**Measured:** 116

**Predicted:** 107

[Image not found](#)

Cyclopropanecarboxylic acid, 1-  
((4-bromophenyl)sulfonyl)-,  
methyl ester

**Measured:** 124

**Predicted:** 110

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Cyclobutanecarboxylic acid, 1-  
((4-chlorophenyl)sulfonyl)-, 1-  
methylethyl ester

**Measured:** 76.2

**Predicted:** 90.9

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Cyclobutanecarboxylic acid, 1-  
((4-bromophenyl)sulfonyl)-,  
methyl ester

**Measured:** 95.0

**Predicted:** 99.6

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Cyclopentanecarboxylic acid, 1-  
((4-bromophenyl)sulfonyl)-,  
methyl ester

**Measured:** 104

**Predicted:** 96.7