

Cyclobutanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester
160790-09-0 | DTXSID20166995

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: 90.9 °C

Global applicability domain: Inside

Local applicability domain index: 8.54e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

[Image not found](#)

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

Measured: 76.2

Predicted: 90.9

[Image not found](#)

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

Measured: 95.0

Predicted: 99.6

[Image not found](#)

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

Measured: 89.8

Predicted: 93.8

[Image not found](#)

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

Measured: 116

Predicted: 107

[Image not found](#)

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

Measured: 104

Predicted: 96.7