

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

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 322 °C

Global applicability domain: Inside

Local applicability domain index: 3.63e-01

Confidence level: 4.92e-01

Nearest Neighbors from the Training Set

Image not found

Benzene, 1,1'-sulfonylbis[4-methyl-

Measured: 406

Predicted: 360

Image not found

Diphenylsulfone

Measured: 279

Predicted: 315

Image not found

1,3-Benzodioxole, 4,7-dimethoxy-5-(2-propenyl)-

Measured: 294

Predicted: 287

Image not found

Benzene, 1,1'-oxybis[2-methoxy-

Measured: 331

Predicted: 310