

Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester
145348-23-8 | DTXSID20162992

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.63e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 3.99e-01

Nearest Neighbors from the Training Set

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Endosulfan sulfate

Measured: 1.14e-06

Predicted: 6.86e-06

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

Measured: 1.00e-03

Predicted: 3.91e-04

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

Measured: 4.91e-04

Predicted: 9.14e-04

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

Measured: 2.88e-04

Predicted: 2.63e-04