

Endosulfan sulfate
1031-07-8 | DTXSID3037541

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 9.29

Global applicability domain: Inside

Local applicability domain index: 9.85e-01

Confidence level: 5.16e-01

Nearest Neighbors from the Training Set

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2,2',3,4,4',5'-Hexachlorobiphenyl

Measured: 9.80

Predicted: 9.29

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2,2',4,4',5,5'-Hexachlorobiphenyl

Measured: 9.73

Predicted: 9.70

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2,2',3,4',5',6'-Hexachlorobiphenyl

Measured: 9.27

Predicted: 9.70

Image not found

2,2',4,4',6,6'-Hexachlorobiphenyl

Measured: 8.99

Predicted: 9.93

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(+/-)-Oxychlorane

Measured: 8.39

Predicted: 9.71