

2,3,6-Trichlorophenylacetic acid sodium salt
2439-00-1 | DTXSID4041319

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.50e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.24e-01

Confidence level: 6.61e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Naphthoquinone

Measured: 3.10e-12

Predicted: 3.16e-11

Image not found

alpha-Angelica lactone

Measured: 6.90e-11

Predicted: 6.33e-11

Image not found

2-Methyl-p-benzoquinone

Measured: 2.35e-11

Predicted: 2.15e-11

Image not found

(3Z)-3-Hexenyl acetate

Measured: 7.80e-11

Predicted: 7.52e-11