

Niridazole
61-57-4 | DTXSID6045244

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.22e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.91e-01

Confidence level: 7.39e-01

Nearest Neighbors from the Training Set

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2-Methylfuran

Measured: 1.20e-04

Predicted: 66.8

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Oxadiargyl

Measured: 3.00e-05

Predicted: 1.54e-08

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4-tert-Butylcyclohexyl acetate

Measured: 1.27e-05

Predicted: 2.32e-02

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2,4-Dinitrophenol

Measured: 3.90e-04

Predicted: 2.01e-04

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Phenyl methyl difluorosilane

Measured: 1.22e-04

Predicted: 2.86