

Pendimethalin
40487-42-1 | DTXSID7024245

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: 335 °C

Global applicability domain: Outside

Local applicability domain index: 2.86e-01

Confidence level: 5.79e-01

Nearest Neighbors from the Training Set

Image not found

Pendimethalin

Measured: 330

Predicted: 335

Image not found

Benfluralin

Measured: 370

Predicted: 349

Image not found

Auramine

Measured: 331

Predicted: 349

Image not found

4-Aminoazobenzene

Measured: 366

Predicted: 337

Image not found

2,3,4-Trinitrotoluene

Measured: 301

Predicted: 309