

Pyrithiobac-sodium
123343-16-8 | DTXSID8032673

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: 332 °C

Global applicability domain: Outside

Local applicability domain index: 1.92e-01

Confidence level: 4.13e-01

Nearest Neighbors from the Training Set

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Benzoic acid, 2-phenylhydrazide

Measured: 314

Predicted: 306

Image not found

2-Acetylamino fluorene

Measured: 303

Predicted: 340

Image not found

2-Acetamidobiphenyl

Measured: 355

Predicted: 321

Image not found

Flurprimidol

Measured: 264

Predicted: 304

Image not found

Dehydrothio-4-toluidine

Measured: 434

Predicted: 377