

Carboxin
5234-68-4 | DTXSID0023951

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 104 °C

Global applicability domain: Inside

Local applicability domain index: 4.96e-01

Confidence level: 5.14e-01

Nearest Neighbors from the Training Set

Image not found

Carboxin

Measured: 91.5

Predicted: 104

Image not found

6,7-dimethoxy-3,4-dihydro-2H-isoquinolin-1-one

Measured: 175

Predicted: 153

Image not found

Thionalide

Measured: 112

Predicted: 108

Image not found

Etobenzanid

Measured: 92.5

Predicted: 105

Image not found

Indobufen

Measured: 183

Predicted: 185