

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: 260 °C

Global applicability domain: Inside

Local applicability domain index: 4.92e-01

Confidence level: 8.40e-01

Nearest Neighbors from the Training Set

Image not found

Benzoyl chloride, 3,4-dichloro-

Measured: 242

Predicted: 251

Image not found

Benzoyl chloride, 4-bromo-

Measured: 246

Predicted: 247

Image not found

1,3-Benzenedicarbonyl
dichloride

Measured: 276

Predicted: 279

Image not found

1,2-Benzenedicarbonyl
dichloride

Measured: 281

Predicted: 279

Image not found

1,4-Benzenedicarbonyl
dichloride

Measured: 258

Predicted: 279