

Model Performance

Model	Data
-------	------

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: 320 °C

Global applicability domain: Inside

Local applicability domain index: 3.42e-01

Confidence level: 5.42e-01

Nearest Neighbors from the Training Set

Image not found

6-Quinolinamine, N,N,2-trimethyl-

Measured: 319

Predicted: 298

Image not found

1H-Imidazole, 2-phenyl-

Measured: 340

Predicted: 314

Image not found

1,2-Diphenylhydrazine

Measured: 309

Predicted: 350

Image not found

4-Nitrosodiphenylamine

Measured: 292

Predicted: 325