

Model Performance

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

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: 63.8 °C

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 3.75e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N,N-Dimethyl-1,2-dithiolan-4-amine

Measured: 177

Predicted: 127

[Image not found](#)

Ethyl N-butylcarbamate

Measured: -22.0

Predicted: 56.5

[Image not found](#)

Pentanenitrile, 4,4-dimethyl-3-oxo-

Measured: 71.0

Predicted: 66.2