

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: 183 °C

Global applicability domain: Outside

Local applicability domain index: 3.32e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

Image not found

Diisopropylnitrosamine

Measured: 195

Predicted: 189

Image not found

N-Nitrodiethylamine

Measured: 207

Predicted: 196

Image not found

N-Nitrosodipropylamine

Measured: 206

Predicted: 192

Image not found

Ethylene glycol dinitrate

Measured: 199

Predicted: 197

Image not found

Boranediamine, 1-fluoro-
N,N,N',N'-tetramethyl-

Measured: 106

Predicted: 121