

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: -135 °C

Global applicability domain: Inside

Local applicability domain index: 5.13e-01

Confidence level: 6.79e-01

Nearest Neighbors from the Training Set

Image not found

HFC-41

Measured: -142

Predicted: -135

Image not found

1,1-Difluoroethane

Measured: -117

Predicted: -124

Image not found

Vinylidene fluoride

Measured: -144

Predicted: -130

Image not found

HFC-143

Measured: -84.0

Predicted: -95.9

Image not found

1,1,1-Trifluoroethane

Measured: -111

Predicted: -106