

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: -107 °C

Global applicability domain: Inside

Local applicability domain index: 6.32e-01

Confidence level: 5.75e-01

Nearest Neighbors from the Training Set

Image not found

Ethanol

Measured: -114

Predicted: -107

Image not found

1-Propanol

Measured: -126

Predicted: -114

Image not found

Allyl alcohol

Measured: -129

Predicted: -109

Image not found

Isopropanol

Measured: -89.5

Predicted: -99.6

Image not found

tert-Butyl hydroperoxide

Measured: -8.00

Predicted: -23.0