

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: 29.0 °C

Global applicability domain: Outside

Local applicability domain index: 5.14e-01

Confidence level: 9.59e-01

Nearest Neighbors from the Training Set

Image not found

Perflenapent

Measured: 29.2

Predicted: 29.0

Image not found

Perflexane

Measured: 56.6

Predicted: 57.0

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Perfluorobutane

Measured: -1.90

Predicted: -1.58

Image not found

Perflisobutane

Measured: 0.0

Predicted: 1.09

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Perfluoroisohexane

Measured: 57.6

Predicted: 57.6