

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: 73.3 °C

Global applicability domain: Outside

Local applicability domain index: 2.72e-01

Confidence level: 7.02e-01

Nearest Neighbors from the Training Set

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Heptanoic acid,
2,2,3,3,4,4,5,5,6,6,7,7-
dodecafluoro-

Measured: 34.0

Predicted: 32.9

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PFOA

Measured: 55.0

Predicted: 53.2

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Sulfluramid

Measured: 96.0

Predicted: 92.5

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1-Nonanol,
2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9-
hexadecafluoro-

Measured: 56.0

Predicted: 54.2

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Hexanedioic acid, 2,2,3,3,4,4,5,5-
octafluoro-

Measured: 134

Predicted: 123