

PUBCHEM_54609806

3698-87-1 | DTXSID60715027

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: 148 °C

Global applicability domain: Inside

Local applicability domain index: 4.56e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methyl alpha-D-glucopyranoside

Measured: 168

Predicted: 163

[Image not found](#)

L-Arabinose

Measured: 158

Predicted: 155

[Image not found](#)

D-Tagatose

Measured: 135

Predicted: 141

[Image not found](#)

D-Glucose

Measured: 133

Predicted: 141

[Image not found](#)

Galactose

Measured: 133

Predicted: 141

[Image not found](#)

alpha-d-glucopyranose

Measured: 133

Predicted: 141