

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 313 °C

Global applicability domain: Outside

Local applicability domain index: 1.51e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Erythritol

Measured: 331

Predicted: 327

[Image not found](#)

Pyrogallol

Measured: 309

Predicted: 292

[Image not found](#)

Triisopropanolamine

Measured: 305

Predicted: 302

[Image not found](#)

2-(Hydroxymethyl)-2-methyl-
1,3-propanediol

Measured: 283

Predicted: 289

[Image not found](#)

Triethanolamine

Measured: 335

Predicted: 326