

Isopropyl beta-D-1-thiogalactopyranoside
367-93-1 | DTXSID6041052

Model Performance

Model	Data
-------	------

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: 132 °C

Global applicability domain: Inside

Local applicability domain index: 4.33e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Isopropyl beta-D-1-thiogalactopyranoside

Measured: 121

Predicted: 132

[Image not found](#)

Methyl alpha-D-glucopyranoside

Measured: 168

Predicted: 163