

Pentaerythritol
115-77-5 | DTXSID2026943

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: 218 °C

Global applicability domain: Inside

Local applicability domain index: 5.26e-01

Confidence level: 4.14e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Pentaerythritol

Measured: 260

Predicted: 218

[Image not found](#)

Erythritol

Measured: 122

Predicted: 138

[Image not found](#)

D-(-)-Lyxose

Measured: 98.5

Predicted: 155

[Image not found](#)

Deoxyglucose

Measured: 147

Predicted: 143