

Tris(2-hydroxyethyl) isocyanurate
839-90-7 | DTXSID4026266

Model Performance

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: 315 °C

Global applicability domain: Outside

Local applicability domain index: 1.16e-01

Confidence level: 4.69e-01

Nearest Neighbors from the Training Set

Image not found

Triisopropanolamine

Measured: 305

Predicted: 302

Image not found

Dinoseb

Measured: 332

Predicted: 328

Image not found

2,2'-[(4-Methylphenyl)imino]diethanol

Measured: 339

Predicted: 310

Image not found

Metaraminol

Measured: 218

Predicted: 257

Image not found

2-Methyl-4,6-dinitrophenol

Measured: 378

Predicted: 352