

Guanidine, N,N"-((iminodi-8,1-octanediy)bis-
13516-27-3 | DTXSID7042015

Model Performance

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

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: 277 °C

Global applicability domain: Outside

Local applicability domain index: 5.81e-02

Confidence level: 6.56e-01

Nearest Neighbors from the Training Set

Image not found

Diphenylurea

Measured: 262

Predicted: 269

Image not found

N-(4-Bromophenyl)urea

Measured: 260

Predicted: 256

Image not found

1-Phenylurea

Measured: 238

Predicted: 247

Image not found

Tetraethylenepentamine

Measured: 342

Predicted: 339

Image not found

2,6-Diaminopyridine

Measured: 285

Predicted: 309