

N-Butyl-3-chloro-6-hydrazinylpyridazin-4-amine
61261-46-9 | DTXSID90615440

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: 332 °C

Global applicability domain: Outside

Local applicability domain index: 1.92e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

Image not found

Desmetryn

Measured: 345

Predicted: 341

Image not found

Ametryn

Measured: 345

Predicted: 341

Image not found

Tetraethylenepentamine

Measured: 342

Predicted: 339

Image not found

Triethylenetetramine

Measured: 267

Predicted: 265

Image not found

1,2,4-Triaminobenzene

Measured: 340

Predicted: 315