

4-Aminopyridine
504-24-5 | DTXSID0023870

Model Performance

Model	Data
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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: 238 °C

Global applicability domain: Inside

Local applicability domain index: 4.56e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

Image not found

4-Methylpyrazole

Measured: 206

Predicted: 201

Image not found

4-chloro-3,5-dimethyl-1H-pyrazole

Measured: 221

Predicted: 242

Image not found

Hexanenitrile, 6-amino-

Measured: 236

Predicted: 236

Image not found

4-Bromopyrazole

Measured: 255

Predicted: 244