

n,n-bis(2-cyanoethyl)aspartic acid  
6328-90-1 | DTXSID20286167

## 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
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** 179 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 3.33e-01

**Confidence level:** 4.02e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Primocarcin

**Measured:** 131

**Predicted:** 143

[Image not found](#)

(4-(2-Hydroxyethyl)-1-piperazineethanesulfonic acid

**Measured:** 234

**Predicted:** 209

[Image not found](#)

Cartap hydrochloride

**Measured:** 180

**Predicted:** 184