

beta-Alanine, N-methyl-
2679-14-3 | DTXSID10181298

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: 216 °C

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 2.83e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-(2-Hydroxyethyl)acetamide

Measured: 16.0

Predicted: 74.9

[Image not found](#)

beta-Aminobutyric acid

Measured: 193

Predicted: 250

[Image not found](#)

Alanine, 2-methyl-

Measured: 335

Predicted: 307