

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 179 °C

Global applicability domain: Inside

Local applicability domain index: 2.61e-01

Confidence level: 6.85e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethoxyacetic acid

Measured: 207

Predicted: 195

[Image not found](#)

3-Chloropropanoic acid

Measured: 156

Predicted: 172

[Image not found](#)

N-Methylcarbamic acid, ethyl ester

Measured: 170

Predicted: 176

[Image not found](#)

2-Chloropropanoic acid

Measured: 185

Predicted: 179

[Image not found](#)

Ethyl ethylcarbamate

Measured: 176

Predicted: 180