

beta-Aminobutyric acid
541-48-0 | DTXSID4040975

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: 186 °C

Global applicability domain: Inside

Local applicability domain index: 2.67e-01

Confidence level: 7.03e-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

Cyclobutanecarboxylic acid

Measured: 190

Predicted: 192

Image not found

2-Chloropropanoic acid

Measured: 185

Predicted: 179

Image not found

Dichloroacetic acid

Measured: 194

Predicted: 191