

Butylamine  
109-73-9 | DTXSID1021904

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:** 68.1 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 8.73e-01

**Confidence level:** 8.01e-01

## Nearest Neighbors from the Training Set

Image not found

Butylamine

**Measured:** 78.0

**Predicted:** 68.1

Image not found

Isobutylamine

**Measured:** 68.5

**Predicted:** 64.1

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2-Butanamine

**Measured:** 62.8

**Predicted:** 63.9

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N-Methyl-N-propylamine

**Measured:** 62.0

**Predicted:** 59.3

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tert-Butylamine

**Measured:** 45.0

**Predicted:** 56.7