

Acetone  
67-64-1 | DTXSID8021482

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:** 48.2 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 7.16e-01

**Confidence level:** 8.16e-01

## Nearest Neighbors from the Training Set

Image not found

Acetone

**Measured:** 55.8

**Predicted:** 48.2

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(2H6)Acetone

**Measured:** 55.8

**Predicted:** 50.0

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Propanal

**Measured:** 48.0

**Predicted:** 47.1

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Methyl formate

**Measured:** 31.7

**Predicted:** 36.7

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1,3-Propylene oxide

**Measured:** 47.6

**Predicted:** 40.7