

Isobutyl nitrite  
542-56-3 | DTXSID3020750

### 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:** 38.3 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 6.01e-01

**Confidence level:** 6.72e-01

## Nearest Neighbors from the Training Set

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Acetamide, N-acetyl-N-methyl-

**Measured:** -25.0

**Predicted:** -28.7

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Acetoxime

**Measured:** 61.0

**Predicted:** 37.2

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2,3-Butanedione-2-oxime

**Measured:** 76.8

**Predicted:** 74.5

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Trimethadione

**Measured:** 46.0

**Predicted:** 51.8