

2-Nitropropane  
79-46-9 | DTXSID6020981

### 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:** -84.6 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 6.81e-01

**Confidence level:** 4.88e-01

## Nearest Neighbors from the Training Set

Image not found

2-Nitropropane

**Measured:** -91.3

**Predicted:** -84.6

Image not found

1-Nitropropane

**Measured:** -108

**Predicted:** -87.7

Image not found

Propane, 2-methyl-1-nitro-

**Measured:** -76.9

**Predicted:** -40.3

Image not found

1-Nitrobutane

**Measured:** -81.3

**Predicted:** -46.4

Image not found

Propane, 2-methyl-2-nitro-

**Measured:** 26.2

**Predicted:** -20.5