

2-Nitrobenzamide  
610-15-1 | DTXSID0025733

### Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

#### Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.84            | 0.55 | 0.85           | 0.53 | 0.83       | 0.64 |

## Model Results

**Predicted value:** 3.83

**Global applicability domain:** Inside

**Local applicability domain index:** 5.24e-01

**Confidence level:** 8.28e-01

## Nearest Neighbors from the Training Set

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2,2-Dimethylpropane-1,3-diol

**Measured:** 4.68

**Predicted:** 4.44

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tert-Butyl alcohol

**Measured:** 5.01

**Predicted:** 4.48

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2,2-Bis(bromomethyl)-1,3-propanediol

**Measured:** 4.79

**Predicted:** 3.35

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Thiourea

**Measured:** 2.00

**Predicted:** 2.11

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Paraldehyde

**Measured:** 3.02

**Predicted:** 2.77