

Furan

110-00-9 | DTXSID6020646

### Model Performance

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

#### Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.81            | 0.55 | 0.81           | 0.54 | 0.71       | 0.61 |

## Model Results

**Predicted value:** 16.3 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.84e-01

**Confidence level:** 7.86e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Epichlorohydrin

**Measured:** 10.0

**Predicted:** 9.87

[Image not found](#)

Pyridine

**Measured:** 39.8

**Predicted:** 20.1

[Image not found](#)

Thioacetamide

**Measured:** 6.03

**Predicted:** 6.43

[Image not found](#)

Benzene

**Measured:** 56.2

**Predicted:** 50.5

[Image not found](#)

Methyl isothiocyanate

**Measured:** 9.33

**Predicted:** 7.63