

1,4-Benzoquinone  
106-51-4 | DTXSID6020145

### 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
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 28.6 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.85e-01

**Confidence level:** 8.29e-01

## Nearest Neighbors from the Training Set

Image not found

3-Pyridinecarbonitrile

**Measured:** 36.3

**Predicted:** 25.0

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Benzamide

**Measured:** 28.8

**Predicted:** 29.7

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Benzoic acid

**Measured:** 31.6

**Predicted:** 35.5

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Benzyl alcohol

**Measured:** 12.6

**Predicted:** 20.1

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2-(Pyridin-2-yl)ethanol

**Measured:** 28.2

**Predicted:** 35.9