

D-(-)-Mandelic acid  
611-71-2 | DTXSID4046523

### 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:** 52.7 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 6.76e-01

**Confidence level:** 6.70e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

(2-Fluorophenyl)urea

**Measured:** 20.9

**Predicted:** 52.8

[Image not found](#)

Urea, (m-fluorophenyl)-

**Measured:** 58.9

**Predicted:** 59.1

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4-Aminobenzoic acid

**Measured:** 316

**Predicted:** 96.6

[Image not found](#)

Urea, (3-methylphenyl)-

**Measured:** 36.3

**Predicted:** 37.2

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Urea, 1-(p-fluorophenyl)-

**Measured:** 33.1

**Predicted:** 49.6