

Aspirin  
50-78-2 | DTXSID5020108

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:** 61.3 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 6.41e-01

**Confidence level:** 6.74e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Metaldehyde acetaldehyde  
tetramer

**Measured:** 240

**Predicted:** 148

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Phthalic acid

**Measured:** 11.7

**Predicted:** 21.4

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Dimethyl phthalate

**Measured:** 39.8

**Predicted:** 59.9

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N-(3-chlorophenyl)-N'-  
methylurea

**Measured:** 85.1

**Predicted:** 101

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[3-(Trifluoromethyl)phenyl]urea

**Measured:** 95.5

**Predicted:** 94.0