

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
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** 1.41

**Global applicability domain:** Inside

**Local applicability domain index:** 6.84e-01

**Confidence level:** 7.26e-01

## Nearest Neighbors from the Training Set

Image not found

Aspirin

**Measured:** 1.19

**Predicted:** 1.41

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Benzoic acid, 4-(acetyloxy)-

**Measured:** 1.48

**Predicted:** 1.27

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3-Acetoxybenzoic acid

**Measured:** 1.49

**Predicted:** 1.42

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Monomethyl phthalate

**Measured:** 1.13

**Predicted:** 1.85

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3-(Methoxycarbonyl)benzoic acid

**Measured:** 1.83

**Predicted:** 1.84