

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
0.95	0.69	0.95	0.65	0.96	0.68

## Model Results

**Predicted value:** 7.72

**Global applicability domain:** Inside

**Local applicability domain index:** 7.03e-01

**Confidence level:** 3.69e-01

## Nearest Neighbors from the Training Set

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Methylparaben

**Measured:** 8.57

**Predicted:** 7.06

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Phenacetin

**Measured:** 9.59

**Predicted:** 9.23

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1-Octanol

**Measured:** 6.03

**Predicted:** 5.95

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Diphenylamine

**Measured:** 7.64

**Predicted:** 8.73

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Cyclohexanol

**Measured:** 5.18

**Predicted:** 4.72