

2-Butanol  
78-92-2 | DTXSID9021762

### 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	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 8.64e-12 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 8.44e-01

**Confidence level:** 6.77e-01

## Nearest Neighbors from the Training Set

Image not found

2-Butanol

**Measured:** 9.60e-12

**Predicted:** 8.64e-12

Image not found

1-Butanol

**Measured:** 8.57e-12

**Predicted:** 1.06e-11

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1,4-Diazabicyclo[2.2.2]octane

**Measured:** 2.20e-11

**Predicted:** 1.30e-11

Image not found

Cyclopentanol

**Measured:** 1.07e-11

**Predicted:** 1.17e-11

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tert-Butyl alcohol

**Measured:** 1.12e-12

**Predicted:** 3.20e-12