

(<sup>13</sup>C<sub>3</sub>)Propan-1-ol  
1173020-91-1 | DTXSID40745923

## 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:** 7.35e-12 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 7.93e-01

**Confidence level:** 7.77e-01

## Nearest Neighbors from the Training Set

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1-Propanol

**Measured:** 5.53e-12

**Predicted:** 7.35e-12

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Isopropanol

**Measured:** 5.07e-12

**Predicted:** 5.72e-12

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1,4-Diazabicyclo[2.2.2]octane

**Measured:** 2.20e-11

**Predicted:** 1.30e-11

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1-Butanol

**Measured:** 8.57e-12

**Predicted:** 1.06e-11

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2-Butanol

**Measured:** 9.60e-12

**Predicted:** 8.64e-12