

2-(propan-2-yl)-1,3,6-trioxocane  
15351-38-9 | DTXSID80279934

## 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:**  $3.77 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $6.74 \times 10^{-1}$

**Confidence level:**  $8.32 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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1-Butoxy-2-propanol

**Measured:**  $3.76 \times 10^{-11}$

**Predicted:**  $3.73 \times 10^{-11}$

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Diethylene glycol diethyl ether

**Measured:**  $2.68 \times 10^{-11}$

**Predicted:**  $2.50 \times 10^{-11}$

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2-(2-Butoxyethoxy)ethanol

**Measured:**  $7.44 \times 10^{-11}$

**Predicted:**  $5.15 \times 10^{-11}$

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3-Methoxybutan-1-ol

**Measured:**  $2.36 \times 10^{-11}$

**Predicted:**  $2.52 \times 10^{-11}$