

Isobutyric anhydride  
97-72-3 | DTXSID7026609

### 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:**  $4.46 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $5.44 \times 10^{-1}$

**Confidence level:**  $7.48 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Dimethyl glutarate

**Measured:**  $3.30 \times 10^{-12}$

**Predicted:**  $3.76 \times 10^{-12}$

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Dimethyl adipate

**Measured:**  $8.40 \times 10^{-12}$

**Predicted:**  $6.84 \times 10^{-12}$

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Dimethyl succinate

**Measured:**  $1.40 \times 10^{-12}$

**Predicted:**  $1.93 \times 10^{-12}$

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Pentyl acetate

**Measured:**  $7.55 \times 10^{-12}$

**Predicted:**  $6.38 \times 10^{-12}$

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Ethyl 3-ethoxypropionate

**Measured:**  $2.29 \times 10^{-11}$

**Predicted:**  $1.63 \times 10^{-11}$