

Acetamide  
60-35-5 | DTXSID7020005

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:**  $1.10 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $5.91 \times 10^{-1}$

**Confidence level:**  $6.75 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Methyl acetate

**Measured:**  $3.41 \times 10^{-13}$

**Predicted:**  $6.02 \times 10^{-13}$

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Ethyl acetate

**Measured:**  $1.60 \times 10^{-12}$

**Predicted:**  $1.92 \times 10^{-12}$

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Propionic acid

**Measured:**  $1.22 \times 10^{-12}$

**Predicted:**  $1.27 \times 10^{-12}$

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N-Methylacetamide

**Measured:**  $5.20 \times 10^{-12}$

**Predicted:**  $3.62 \times 10^{-12}$

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Methyl propanoate

**Measured:**  $1.00 \times 10^{-12}$

**Predicted:**  $1.63 \times 10^{-12}$