

Ethylene  
74-85-1 | DTXSID1026378

### 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:**  $9.54 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $2.63 \times 10^{-1}$

**Confidence level:**  $8.18 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Ethylene

**Measured:**  $8.52 \times 10^{-12}$

**Predicted:**  $9.54 \times 10^{-12}$

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1,2-Propadiene

**Measured:**  $9.84 \times 10^{-12}$

**Predicted:**  $1.07 \times 10^{-11}$

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1-Propene

**Measured:**  $2.63 \times 10^{-11}$

**Predicted:**  $2.80 \times 10^{-11}$

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1-Butene

**Measured:**  $3.14 \times 10^{-11}$

**Predicted:**  $3.13 \times 10^{-11}$

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3-Methyl-1-butene

**Measured:**  $3.18 \times 10^{-11}$

**Predicted:**  $3.27 \times 10^{-11}$