

Pentane  
109-66-0 | DTXSID2025846

### 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:**  $4.10 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $8.08 \times 10^{-1}$

**Confidence level:**  $9.09 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Pentane

**Measured:**  $3.94 \times 10^{-12}$

**Predicted:**  $4.10 \times 10^{-12}$

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2-Methylbutane

**Measured:**  $3.90 \times 10^{-12}$

**Predicted:**  $4.63 \times 10^{-12}$

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n-Hexane

**Measured:**  $5.61 \times 10^{-12}$

**Predicted:**  $5.55 \times 10^{-12}$

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Butane

**Measured:**  $2.54 \times 10^{-12}$

**Predicted:**  $2.53 \times 10^{-12}$

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2,3-Dimethylbutane

**Measured:**  $6.20 \times 10^{-12}$

**Predicted:**  $4.81 \times 10^{-12}$