

Heptane  
142-82-5 | DTXSID6024127

### 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:**  $6.52 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $9.02 \times 10^{-1}$

**Confidence level:**  $9.43 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Heptane

**Measured:**  $7.15 \times 10^{-12}$

**Predicted:**  $6.52 \times 10^{-12}$

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3-Methylpentane

**Measured:**  $5.70 \times 10^{-12}$

**Predicted:**  $5.37 \times 10^{-12}$

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2-Methylpentane

**Measured:**  $5.60 \times 10^{-12}$

**Predicted:**  $5.41 \times 10^{-12}$

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Octane

**Measured:**  $8.68 \times 10^{-12}$

**Predicted:**  $7.74 \times 10^{-12}$

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n-Hexane

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

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