

Myrcene  
123-35-3 | DTXSID6025692

Model Performance

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:** 2.05e-10 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 2.98e-01

**Confidence level:** 9.11e-01

## Nearest Neighbors from the Training Set

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Myrcene

**Measured:** 2.15e-10

**Predicted:** 2.05e-10

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Ocimene (E)

**Measured:** 2.52e-10

**Predicted:** 2.40e-10

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beta-Ocimene

**Measured:** 2.52e-10

**Predicted:** 2.40e-10

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2-Methylhexa-1,5-diene

**Measured:** 9.60e-11

**Predicted:** 9.53e-11

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1,5-Hexadiene, 2,5-dimethyl-

**Measured:** 1.20e-10

**Predicted:** 1.18e-10

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D-Limonene

**Measured:** 1.71e-10

**Predicted:** 1.73e-10