

4-(1-Cyanoethyl)-1,2,3,4-tetrahydronaphthalene-1-carbonitrile  
57964-39-3 | DTXSID2057576

### 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:** 1.13e-10 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 1.97e-01

**Confidence level:** 8.63e-01

## Nearest Neighbors from the Training Set

Image not found

alpha-Phellandrene

**Measured:** 3.13e-10

**Predicted:** 2.83e-10

Image not found

alpha-Humulene

**Measured:** 2.90e-10

**Predicted:** 2.87e-10

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(3Z)-3-Hexenyl acetate

**Measured:** 7.80e-11

**Predicted:** 7.52e-11

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Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

**Measured:** 4.80e-11

**Predicted:** 4.73e-11

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(2E)-2-Hexenal

**Measured:** 4.40e-11

**Predicted:** 4.31e-11