

Nitromethane  
75-52-5 | DTXSID2020977

### 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:** 1.51e-13 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 4.94e-01

**Confidence level:** 6.73e-01

## Nearest Neighbors from the Training Set

Image not found

Nitromethane

**Measured:** 1.30e-13

**Predicted:** 1.51e-13

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Methyl nitrite

**Measured:** 2.20e-13

**Predicted:** 2.32e-13

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Ethyl nitrate

**Measured:** 2.00e-13

**Predicted:** 3.49e-13

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Methyl nitrate

**Measured:** 3.50e-13

**Predicted:** 3.14e-13

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Nitroethane

**Measured:** 1.50e-13

**Predicted:** 3.42e-13