

Acetic acid, trifluoro-, methyl ester  
431-47-0 | DTXSID2059988

### 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:** 5.42e-14 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 3.04e-01

**Confidence level:** 5.46e-01

## Nearest Neighbors from the Training Set

Image not found

Acetic acid, trifluoro-, methyl ester

**Measured:** 5.20e-14

**Predicted:** 5.42e-14

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2-Propanone, 1,1,1-trifluoro-

**Measured:** 1.51e-14

**Predicted:** 2.15e-14

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Acetic acid, trifluoro-

**Measured:** 1.20e-13

**Predicted:** 1.81e-13

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Hexafluorobenzene

**Measured:** 1.71e-13

**Predicted:** 6.65e-14

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Peroxyacetyl nitrate

**Measured:** 1.00e-13

**Predicted:** 9.98e-14