

2,2,2-Trifluoroethanol  
75-89-8 | DTXSID0021751

### 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:** 4.61e-14 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 6.31e-01

**Confidence level:** 6.69e-01

## Nearest Neighbors from the Training Set

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2,2,2-Trifluoroethanol

**Measured:** 9.55e-14

**Predicted:** 4.61e-14

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1,1,1,3,3-Pentafluoropropane

**Measured:** 7.28e-15

**Predicted:** 1.06e-14

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Bromotrifluoroethane

**Measured:** 2.05e-14

**Predicted:** 2.07e-14

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1,2-Dichloro-1,1-difluoroethane

**Measured:** 1.60e-14

**Predicted:** 1.99e-14

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Ethane, 2-(difluoromethoxy)-  
1,1,1-trifluoro-

**Measured:** 1.20e-14

**Predicted:** 2.17e-14