

Sulfone, methyl pentafluorophenyl  
651-85-4 | DTXSID30215403

## 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:**  $2.18 \times 10^{-13}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $1.62 \times 10^{-1}$

**Confidence level:**  $6.32 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Peroxyacetyl nitrate

**Measured:**  $1.00 \times 10^{-13}$

**Predicted:**  $9.98 \times 10^{-14}$

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Propylene dinitrate

**Measured:**  $3.20 \times 10^{-13}$

**Predicted:**  $3.59 \times 10^{-13}$

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Dimethyl sulfate

**Measured:**  $5.00 \times 10^{-13}$

**Predicted:**  $4.96 \times 10^{-13}$

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Diethyl sulfate

**Measured:**  $1.80 \times 10^{-12}$

**Predicted:**  $1.55 \times 10^{-12}$

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

**Measured:**  $1.51 \times 10^{-14}$

**Predicted:**  $2.15 \times 10^{-14}$