

Ethyl perfluoropropionate
426-65-3 | DTXSID2059980

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: 1.05×10^{-13} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.64×10^{-1}

Confidence level: 5.41×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Acetic acid, trifluoro-, methyl ester

Measured: 5.20×10^{-14}

Predicted: 5.42×10^{-14}

Image not found

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

Measured: 1.51×10^{-14}

Predicted: 2.15×10^{-14}

Image not found

Acetic acid, trifluoro-

Measured: 1.20×10^{-13}

Predicted: 1.81×10^{-13}

Image not found

Peroxyacetyl nitrate

Measured: 1.00×10^{-13}

Predicted: 9.98×10^{-14}