

Methyl pivalate
598-98-1 | DTXSID4027234

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: 2.87×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.76×10^{-1}

Confidence level: 6.84×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Isobutyl acetate

Measured: 5.50×10^{-12}

Predicted: 5.09×10^{-12}

Image not found

tert-Butyl acetate

Measured: 4.50×10^{-13}

Predicted: 1.47×10^{-12}

Image not found

Methyl butyrate

Measured: 3.04×10^{-12}

Predicted: 3.29×10^{-12}

Image not found

Butan-2-yl acetate

Measured: 5.50×10^{-12}

Predicted: 5.07×10^{-12}

Image not found

Butyl acetate

Measured: 4.90×10^{-12}

Predicted: 4.91×10^{-12}