

Acetone
67-64-1 | DTXSID8021482

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: 4.07×10^{-13} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.13×10^{-1}

Confidence level: 6.93×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Acetone

Measured: 2.19×10^{-13}

Predicted: 4.07×10^{-13}

Image not found

Cyclobutanone

Measured: 8.70×10^{-13}

Predicted: 1.01×10^{-12}

Image not found

Methyl ethyl ketone

Measured: 1.15×10^{-12}

Predicted: 1.50×10^{-12}

Image not found

Cyclopentanone

Measured: 2.94×10^{-12}

Predicted: 2.41×10^{-12}

Image not found

3-Pentanone

Measured: 2.00×10^{-12}

Predicted: 2.29×10^{-12}