

Methyl acetate
79-20-9 | DTXSID4021767

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: 6.02e-13 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

Image not found

Methyl acetate

Measured: 3.41e-13

Predicted: 6.02e-13

Image not found

Ethyl acetate

Measured: 1.60e-12

Predicted: 1.92e-12

Image not found

Methyl propanoate

Measured: 1.00e-12

Predicted: 1.63e-12

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N-Methylacetamide

Measured: 5.20e-12

Predicted: 3.62e-12

Image not found

Propionic acid

Measured: 1.22e-12

Predicted: 1.27e-12