

1-Octanol
111-87-5 | DTXSID7021940

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: 1.66e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.94e-01

Confidence level: 7.74e-01

Nearest Neighbors from the Training Set

Image not found

1-Octanol

Measured: 1.44e-11

Predicted: 1.66e-11

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1-Heptanol

Measured: 1.37e-11

Predicted: 1.45e-11

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2,4-Dimethylpentan-2-ol

Measured: 1.14e-11

Predicted: 1.35e-11

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Dibutyl sulfide

Measured: 3.74e-11

Predicted: 1.95e-11

Image not found

Butyl ether

Measured: 2.88e-11

Predicted: 2.21e-11