

1-Eicosanol
629-96-9 | DTXSID0027272

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.03e-08 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.35e-01

Confidence level: 5.08e-01

Nearest Neighbors from the Training Set

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1-Octadecanol

Measured: 4.07e-09

Predicted: 1.32e-08

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Heptadecan-1-ol

Measured: 3.12e-08

Predicted: 4.13e-08

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1-Hexadecanol

Measured: 9.69e-08

Predicted: 9.67e-08

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Docosanoic acid

Measured: 4.70e-08

Predicted: 5.44e-08

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Octadecanoic acid

Measured: 2.10e-06

Predicted: 7.52e-07