

Isopropanol

67-63-0 | DTXSID7020762

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)

Training (75%)

Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 7.53 days

Global applicability domain: Outside

Local applicability domain index: 4.18e-01

Confidence level: 8.85e-01

Nearest Neighbors from the Training Set

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Pentane

Measured: 5.00

Predicted: 6.52

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n-Hexane

Measured: 9.00

Predicted: 7.45

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Heptane

Measured: 7.00

Predicted: 7.54

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Octane

Measured: 9.00

Predicted: 8.57

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Nonane

Measured: 9.00

Predicted: 8.49