

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.38e-01

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 6.71e-01

Nearest Neighbors from the Training Set

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1-Propanol

Measured: 0.48

Predicted: 6.71e-01

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Ethanol

Measured: 0.2

Predicted: 3.50e-01

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Thioacetamide

Measured: 0.78

Predicted: 8.08e-01

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Ethyleneimine

Measured: 0.78

Predicted: 6.20e-01

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Acetic acid

Measured: 0.0

Predicted: 3.79e-01