

Isopropyl beta-D-1-thiogalactopyranoside
367-93-1 | DTXSID6041052

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.42e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 2.85e-01

Confidence level: 2.75e-01

Nearest Neighbors from the Training Set

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Dibenzofuran, 1,2,3,4,8-pentachloro-

Measured: 2.84e-11

Predicted: 2.10e-09

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2,4,5-Trimethylphenol

Measured: 7.50e-08

Predicted: 1.72e-02

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Atrazine

Measured: 7.21e-11

Predicted: 2.03e-07

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L-Glutamic acid

Measured: 1.70e-08

Predicted: 1.68e-08

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Nicotine

Measured: 5.28e-09

Predicted: 3.96e-03