

Methyl alpha-D-glucopyranoside
97-30-3 | DTXSID7026605

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: 2.36e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 2.91e-01

Confidence level: 2.99e-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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Lepidine

Measured: 8.02e-14

Predicted: 9.90e-03

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Benz(a)anthracene

Measured: 1.97e-10

Predicted: 2.14e-08

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L-Glutamic acid

Measured: 1.70e-08

Predicted: 1.68e-08