

Ethyl 1-thio-beta-D-galactopyranoside
56245-60-4 | DTXSID70440378

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: 8.32e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 2.94e-01

Confidence level: 3.43e-01

Nearest Neighbors from the Training Set

Image not found

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

Measured: 2.84e-11

Predicted: 2.10e-09

Image not found

2,4,5-Trimethylphenol

Measured: 7.50e-08

Predicted: 1.72e-02

Image not found

L-Glutamic acid

Measured: 1.70e-08

Predicted: 1.68e-08

Image not found

Atrazine

Measured: 7.21e-11

Predicted: 2.03e-07

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Benz(a)anthracene

Measured: 1.97e-10

Predicted: 2.14e-08