

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.17 days

Global applicability domain: Outside

Local applicability domain index: 2.14e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

Image not found

9-Ethyl-9H-fluorene

Measured: 2330

Predicted: N/A

Image not found

5-Methylindan

Measured: 4.93

Predicted: 2.25

Image not found

4-Methylindan

Measured: 4.93

Predicted: 2.31

Image not found

1H-Indene, 2-methyl-

Measured: 12.5

Predicted: 2.48

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17