

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.31

Global applicability domain: Inside

Local applicability domain index: 6.83e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl 1-thio-beta-D-galactopyranoside

Measured: -1.51

Predicted: -1.31

[Image not found](#)

Isopropyl beta-D-1-thiogalactopyranoside

Measured: -1.26

Predicted: -1.16

[Image not found](#)

NSC226971

Measured: -0.630

Predicted: -0.623

[Image not found](#)

Dibromomannitol

Measured: -0.240

Predicted: -0.498

[Image not found](#)

Dibromodulcitol

Measured: -0.240

Predicted: -0.498