

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 41.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.90e-01

Confidence level: 5.26e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Endothal

Measured: 123

Predicted: 109

[Image not found](#)

Cymoxanil

Measured: 123

Predicted: 72.0

[Image not found](#)

Monocrotophos

Measured: 1.00

Predicted: 2.76

[Image not found](#)

Phenazopyridine

Measured: 209

Predicted: 268

[Image not found](#)

Asulam

Measured: 39.8

Predicted: 38.8