

Isopropyl beta-D-1-thiogalactopyranoside
367-93-1 | DTXSID6041052

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: 42.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.70e-01

Confidence level: 5.13e-01

Nearest Neighbors from the Training Set

Image not found

Endothal

Measured: 123

Predicted: 109

Image not found

Monocrotophos

Measured: 1.00

Predicted: 2.76

Image not found

Phenazopyridine

Measured: 209

Predicted: 268

Image not found

Cymoxanil

Measured: 123

Predicted: 72.0

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Dioxacarb

Measured: 39.8

Predicted: 124