

Sucralose

56038-13-2 | DTXSID1040245

Model Performance

Model

Data

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: -0.676

Global applicability domain: Inside

Local applicability domain index: 3.85e-01

Confidence level: 5.48e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Chloralose

Measured: 1.02

Predicted: 5.55e-01

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Isopropyl beta-D-1-thiogalactopyranoside

Measured: -1.26

Predicted: -1.16

[Image not found](#)

Ethyl 1-thio-beta-D-galactopyranoside

Measured: -1.51

Predicted: -1.31

[Image not found](#)

NSC226971

Measured: -0.630

Predicted: -0.623