

Bisphenol A

80-05-7 | DTXSID7020182

Model Performance

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: 3.20

Global applicability domain: Inside

Local applicability domain index: 5.50e-01

Confidence level: 7.84e-01

Nearest Neighbors from the Training Set

Image not found

Bisphenol A

Measured: 3.32

Predicted: 3.20

Image not found

4-Cyclohexylphenylacetic acid

Measured: 3.91

Predicted: 3.90