

MLS000736649
6640-53-5 | DTXSID10287108

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: 3.51

Global applicability domain: Inside

Local applicability domain index: 4.79e-01

Confidence level: 6.35e-01

Nearest Neighbors from the Training Set

Image not found

Phenoxazine

Measured: 3.85

Predicted: 2.99