

1,2-Dichlorobenzene
95-50-1 | DTXSID6020430

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: 398 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.73e-01

Confidence level: 9.19e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Dichlorobenzene

Measured: 363

Predicted: 398

Image not found

1,3-Dichlorobenzene

Measured: 380

Predicted: 400

Image not found

3,5-Dichlorophenol

Measured: 676

Predicted: 319

Image not found

Bromobenzene

Measured: 309

Predicted: 333

Image not found

1,4-Dichlorobenzene

Measured: 447

Predicted: 478