

Phenol, 2,2'-methylenebis[4-methyl-
3236-63-3 | DTXSID0062923

Model Performance

Model	Data
-------	------

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: 455 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.39e-01

Confidence level: 4.98e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl 1-naphthaleneacetate

Measured: 302

Predicted: 425

Image not found

Carbofuran

Measured: 56.2

Predicted: 110

Image not found

3,3'-Dichlorobenzidine

Measured: 22400

Predicted: 1680

Image not found

Isopropylpropylamide

Measured: 148

Predicted: 173

Image not found

Bendiocarb

Measured: 562

Predicted: 247