

4-Hexylresorcinol
136-77-6 | DTXSID1020699

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: 267 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.91e-01

Confidence level: 6.90e-01

Nearest Neighbors from the Training Set

Image not found

MCPB

Measured: 537

Predicted: 245

Image not found

Phenylcarbamic acid butyl ester

Measured: 182

Predicted: 210

Image not found

N-Pentyl N-phenylcarbamate

Measured: 407

Predicted: 375

Image not found

N-Cyclopentyl-N'-phenylurea

Measured: 85.1

Predicted: 122

Image not found

Promecarb

Measured: 302

Predicted: 116