

2,2,4-Trimethyl-1,3-pentanediol
144-19-4 | DTXSID8027113

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: 38.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.32e-01

Confidence level: 8.37e-01

Nearest Neighbors from the Training Set

Image not found

N-Methylbenzamide

Measured: 47.9

Predicted: 53.6

Image not found

Benzamide, 4-methyl-

Measured: 60.3

Predicted: 48.4

Image not found

Phenylacetic acid

Measured: 28.2

Predicted: 43.1

Image not found

Acetanilide

Measured: 26.9

Predicted: 40.2

Image not found

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2