

Heptanedioic acid
111-16-0 | DTXSID5021598

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: 52.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.83e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

Image not found

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

Image not found

N-(3-chlorophenyl)-N'-methylurea

Measured: 85.1

Predicted: 101

Image not found

Urea, 1-(p-fluorophenyl)-

Measured: 33.1

Predicted: 49.6

Image not found

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2

Image not found

Metaldehyde acetaldehyde tetramer

Measured: 240

Predicted: 148