

2,2-Dimethylpentanedioic acid
681-57-2 | DTXSID6021585

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: 45.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

Image not found

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2

Image not found

N-Methyl-N¹-phenylurea

Measured: 19.5

Predicted: 29.8

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Metaldehyde acetaldehyde
tetramer

Measured: 240

Predicted: 148

Image not found

Urea, (m-fluorophenyl)-

Measured: 58.9

Predicted: 59.1

Image not found

(2-Fluorophenyl)urea

Measured: 20.9

Predicted: 52.8