

Butanedioic acid, 2,2,3,3-tetrafluoro-
377-38-8 | DTXSID8059928

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: 41.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.65e-01

Confidence level: 7.30e-01

Nearest Neighbors from the Training Set

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Clopyralid

Measured: 36.3

Predicted: 37.7

Image not found

6-Chloro-2-picolinic acid

Measured: 23.4

Predicted: 53.1

Image not found

Phthalic acid

Measured: 11.7

Predicted: 21.4

Image not found

Tioclorim [ISO]

Measured: 120

Predicted: 93.2

Image not found

3-Bromophenylurea

Measured: 132

Predicted: 114