

Butanamide, 4-hydroxy-
927-60-6 | DTXSID5061297

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: 5.75 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 6.59e-01

Nearest Neighbors from the Training Set

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Diethanolamine

Measured: 3.98

Predicted: 4.00

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1,2-Diethylhydrazine

Measured: 15.1

Predicted: 14.1

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Maleic hydrazide

Measured: 2.82

Predicted: 5.12

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1,2-Propylene glycol

Measured: 2.29

Predicted: 4.24

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1,4-Dioxane

Measured: 17.0

Predicted: 13.2