

Butyl nitrate
928-45-0 | DTXSID70239143

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: 40.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.63e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

Image not found

Anisole

Measured: 34.7

Predicted: 69.5

Image not found

Benzyl alcohol

Measured: 12.6

Predicted: 20.1

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4-Vinylpyridine

Measured: 15.1

Predicted: 43.8

Image not found

p-Cresol

Measured: 501

Predicted: 95.9

Image not found

2-Methoxyphenol

Measured: 36.3

Predicted: 41.2