

N-Butyl nitrite
544-16-1 | DTXSID8049418

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: 27.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.62e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

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1-Pentanol

Measured: 5.01

Predicted: 7.31

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Anisole

Measured: 34.7

Predicted: 69.5

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p-Cresol

Measured: 501

Predicted: 95.9

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4-Vinylpyridine

Measured: 15.1

Predicted: 43.8

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Benzyl alcohol

Measured: 12.6

Predicted: 20.1