

1-Butanol, 3-methoxy-3-methyl-, acetate
103429-90-9 | DTXSID30145852

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: 54.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.62e-01

Confidence level: 7.97e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

[Image not found](#)

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2

[Image not found](#)

N-(3-chlorophenyl)-N'-methylurea

Measured: 85.1

Predicted: 101

[Image not found](#)

Ethyl hexanoate

Measured: 115

Predicted: 110

[Image not found](#)

Ethyl valerate

Measured: 93.3

Predicted: 68.6