

Butyl 3-methoxypropionate
4195-88-4 | DTXSID30194709

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 7.23e-01

Global applicability domain: Inside

Local applicability domain index: 5.73e-01

Confidence level: 7.79e-01

Nearest Neighbors from the Training Set

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1-Methoxy-2-propyl acetate

Measured: 0.56

Predicted: 4.87e-01

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2,2-Dimethyl-1,3-dioxolane

Measured: 0.46

Predicted: 5.11e-01

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Ethyl orthoformate

Measured: 1.20

Predicted: 1.05

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2-(2-Butoxyethoxy)ethanol

Measured: 0.56

Predicted: 5.85e-01

Image not found

Acetal

Measured: 0.84

Predicted: 8.05e-01