

Butanoic acid, propyl ester
105-66-8 | DTXSID6059318

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.45e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.17e-01

Confidence level: 8.97e-01

Nearest Neighbors from the Training Set

Image not found

Butyl propionate

Measured: 1.15e-02

Predicted: 1.44e-02

Image not found

Ethyl isovalerate

Measured: 1.85e-02

Predicted: 1.54e-02

Image not found

Ethyl valerate

Measured: 1.70e-02

Predicted: 1.54e-02

Image not found

Propanoic acid, 2-methylpropyl ester

Measured: 1.31e-02

Predicted: 1.42e-02

Image not found

3-Methylbutyl acetate

Measured: 1.54e-02

Predicted: 1.47e-02