

Propanoic acid, 3-ethoxy-, propyl ester
14144-34-4 | DTXSID9074519

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: 4.53e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.70e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

Image not found

Butyl 3-methoxypropionate

Measured: 6.12e-02

Predicted: 6.04e-02

Image not found

Methyl 3-butoxypropanoate

Measured: 5.12e-02

Predicted: 5.88e-02

Image not found

2-Butoxyethyl acetate

Measured: 5.62e-02

Predicted: 6.06e-02

Image not found

3-Methoxybutyl acetate

Measured: 3.15e-02

Predicted: 1.41e-01

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propyl 3-propoxypropanoate

Measured: 2.07e-02

Predicted: 3.66e-02