

2-Ethoxyethyl acetate
111-15-9 | DTXSID9021928

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: 22.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.59e-01

Confidence level: 5.55e-01

Nearest Neighbors from the Training Set

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1-Methoxy-2-propyl acetate

Measured: 2.29

Predicted: 7.33

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2-Butoxyethanol

Measured: 67.6

Predicted: 45.0

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2-(Pyridin-2-yl)ethanol

Measured: 28.2

Predicted: 35.9

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Urea, 1-(p-fluorophenyl)-

Measured: 33.1

Predicted: 49.6

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4-Aminobenzoic acid

Measured: 316

Predicted: 96.6