

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

Model Performance

Model	Data
-------	------

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: 66.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.36e-01

Confidence level: 7.28e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl valerate

Measured: 93.3

Predicted: 68.6

Image not found

Hexanoic acid

Measured: 28.8

Predicted: 31.6

Image not found

1-Heptanol

Measured: 13.8

Predicted: 18.6

Image not found

Ethyl hexanoate

Measured: 115

Predicted: 110

Image not found

2-Butoxyethanol

Measured: 67.6

Predicted: 45.0