

Isophorone
78-59-1 | DTXSID8020759

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: 103 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.88e-01

Confidence level: 5.82e-01

Nearest Neighbors from the Training Set

Image not found

Isophorone

Measured: 25.1

Predicted: 103

Image not found

1,2,4,5-Tetramethylbenzene

Measured: 1320

Predicted: 1510

Image not found

2,3,5-Trimethylphenol

Measured: 4070

Predicted: 345

Image not found

1,2,3-Trimethylbenzene

Measured: 631

Predicted: 691

Image not found

1,3,5-Trimethylbenzene

Measured: 661

Predicted: 493