

Ethyl hydroperoxide
3031-74-1 | DTXSID70184402

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.286

Global applicability domain: Inside

Local applicability domain index: 5.65e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found

Ethanol

Measured: -0.310

Predicted: -0.276

Image not found

2-Fluoroethanol

Measured: -0.670

Predicted: -0.450

Image not found

Propanol, 3-fluoro-

Measured: -0.280

Predicted: -0.00652

Image not found

1-Propanol

Measured: 0.25

Predicted: 1.27e-01

Image not found

2-Propanol, 1,3-difluoro-

Measured: -0.360

Predicted: -0.0748