

Ethylene oxide
75-21-8 | DTXSID0020600

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -113 °C

Global applicability domain: Inside

Local applicability domain index: 7.26e-01

Confidence level: 6.99e-01

Nearest Neighbors from the Training Set

Image not found

Ethylene oxide

Measured: -112

Predicted: -113

Image not found

1,2-Propylene oxide

Measured: -112

Predicted: -105

Image not found

1,3-Propylene oxide

Measured: -97.0

Predicted: -102

Image not found

Acetaldehyde

Measured: -123

Predicted: -112

Image not found

1,2-Epoxy-3-butene

Measured: -135

Predicted: -115