

Diethylene glycol diethyl ether
112-36-7 | DTXSID3025047

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: 3.03e-01

Global applicability domain: Inside

Local applicability domain index: 5.25e-01

Confidence level: 7.78e-01

Nearest Neighbors from the Training Set

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Diethylene glycol diethyl ether

Measured: 0.39

Predicted: 3.03e-01

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Ethylene glycol diethyl ether

Measured: 0.66

Predicted: 6.93e-01

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1,4,7,10-Tetraoxacyclododecane

Measured: -0.0400

Predicted: -0.0349

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Bis(2-methoxyethyl) ether

Measured: -0.360

Predicted: -0.298