

Diethyl sulfate
64-67-5 | DTXSID1024045

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 3.86

Global applicability domain: Inside

Local applicability domain index: 9.68e-01

Confidence level: 7.37e-01

Nearest Neighbors from the Training Set

Image not found

Tetrachloroethylene

Measured: 3.48

Predicted: 3.86

Image not found

Butyl ether

Measured: 3.89

Predicted: 3.93

Image not found

Ethylbenzene

Measured: 3.74

Predicted: 3.87

Image not found

Nonene

Measured: 3.83

Predicted: 3.95

Image not found

Benzonitrile

Measured: 4.46

Predicted: 3.95