

Acetic acid
64-19-7 | DTXSID5024394

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: -0.136

Global applicability domain: Inside

Local applicability domain index: 5.35e-01

Confidence level: 8.55e-01

Nearest Neighbors from the Training Set

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Acetic acid

Measured: -0.170

Predicted: -0.136

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Propionic acid

Measured: 0.33

Predicted: 4.32e-01

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Propanedioic acid

Measured: -0.810

Predicted: -0.881

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Acrylic acid

Measured: 0.35

Predicted: 3.62e-01

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Urethane

Measured: -0.150

Predicted: -0.120