

Propanoic acid, 2-(1-oxopropoxy)-, methyl ester
61402-72-0 | DTXSID30485366

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.09e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.35e-01

Confidence level: 8.72e-01

Nearest Neighbors from the Training Set

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1,2-Phenylenediamine

Measured: 4.14e-01

Predicted: 8.53e-04

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4-Bromophenol

Measured: 4.10e-01

Predicted: 2.33e-02

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Acetic acid, chloro-, 1-methylethyl ester

Measured: 2.69e-01

Predicted: 6.23

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Benzene, (iodomethyl)-

Measured: 3.00e-01

Predicted: 1.97e-01

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1,3-Diethenylbenzene

Measured: 9.00e-01

Predicted: 8.63e-01