

Methyl hexanedioate
627-91-8 | DTXSID9044451

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.09

Global applicability domain: Inside

Local applicability domain index: 3.45e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

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Benzoic acid, 4-(methylamino)-

Measured: 2.40

Predicted: 4.00

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2,2-Dimethylpropanoic acid

Measured: 2.29

Predicted: 2.74

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3-Nitrobenzoic acid

Measured: 7.08

Predicted: 3.63

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Dalapon-sodium

Measured: 7.24

Predicted: 5.61

Image not found

Phenylphosphinic acid

Measured: 6.03

Predicted: 4.42