

2-ISOPROPYLSUCCINIC ACID
2338-45-6 | DTXSID30281047

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 92.2 °C

Global applicability domain: Inside

Local applicability domain index: 8.78e-01

Confidence level: 6.42e-01

Nearest Neighbors from the Training Set

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2,2-Dimethylpentanedioic acid

Measured: 84.0

Predicted: 90.5

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Pentanedioic acid, 3,3-dimethyl-

Measured: 104

Predicted: 96.7

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2-METHYLHEXANEDIOIC ACID

Measured: 64.0

Predicted: 90.6

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3-Ethyl-3-methylglutaric acid

Measured: 87.0

Predicted: 88.7

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Octanedioic acid

Measured: 144

Predicted: 115