

Acrolein

107-02-8 | DTXSID5020023

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 62.4 °C

Global applicability domain: Inside

Local applicability domain index: 6.40e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

Image not found

Acrolein

Measured: 52.6

Predicted: 62.4

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Methacrylaldehyde

Measured: 68.4

Predicted: 74.5

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(E)-Crotonaldehyde

Measured: 103

Predicted: 91.4

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Crotonaldehyde

Measured: 103

Predicted: 91.4

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2-Methylpropanal

Measured: 64.5

Predicted: 67.6

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Methyl ethyl ketone

Measured: 79.5

Predicted: 72.4