

Acetaldehyde
75-07-0 | DTXSID5039224

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: 682 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.33e-01

Confidence level: 5.70e-01

Nearest Neighbors from the Training Set

Image not found

Acetonitrile

Measured: 902

Predicted: 61.0

Image not found

1,2-Propadiene

Measured: 10400

Predicted: 1730

Image not found

Arecoline

Measured: 232

Predicted: 1.33e-01

Image not found

Dodecylbenzene

Measured: 317

Predicted: 7.09e-05

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3,3-dichloro-1,1,1,2,2-pentafluoropropane

Measured: 63.4

Predicted: 483