

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
26946-56-5 | DTXSID10447169

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 5.27

Global applicability domain: Inside

Local applicability domain index: 9.52e-01

Confidence level: 7.30e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Dibromobenzene

Measured: 5.21

Predicted: 5.09

Image not found

Naphthalene

Measured: 5.19

Predicted: 5.07

Image not found

1,3,5-Trichlorobenzene

Measured: 4.85

Predicted: 5.06

Image not found

1,2,4-Trichlorobenzene

Measured: 4.95

Predicted: 5.06

Image not found

Hexamethylbenzene

Measured: 6.31

Predicted: 5.75