

Oxazole
288-42-6 | DTXSID70182983

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: 2.80

Global applicability domain: Inside

Local applicability domain index: 9.95e-01

Confidence level: 7.35e-01

Nearest Neighbors from the Training Set

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Formic acid, propyl ester

Measured: 2.66

Predicted: 2.80

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Methyl ethyl ketone

Measured: 2.71

Predicted: 2.80

Image not found

Ethyl acetate

Measured: 2.70

Predicted: 2.70

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(Z)-1,2-Dichloroethylene

Measured: 2.56

Predicted: 2.81

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Butyraldehyde

Measured: 3.39

Predicted: 2.81