

1,4-Diazabicyclo[2.2.2]octane
280-57-9 | DTXSID0022016

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.54 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.44e-01

Confidence level: 7.62e-01

Nearest Neighbors from the Training Set

Image not found

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Measured: 4.01

Predicted: 5.54

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4-Methylmorpholine

Measured: 9.89

Predicted: 9.71

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N-Ethylmorpholine

Measured: 8.68

Predicted: 6.40

Image not found

Morpholine

Measured: 11.5

Predicted: 10.8

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N,N'-Dimethylthiourea

Measured: 9.60

Predicted: 5.74