

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 4.25 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.63e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

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Acetic acid

Measured: 1.00

Predicted: 2.40

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Thioacetamide

Measured: 6.03

Predicted: 6.43

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Epichlorohydrin

Measured: 10.0

Predicted: 9.87

Image not found

Methyl isothiocyanate

Measured: 9.33

Predicted: 7.63

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2,2'-Bioxirane

Measured: 2.51

Predicted: 4.97