

2-(Methylsulfonyl)quinoxaline
21948-73-2 | DTXSID00325902

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: 98.9 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.57e-01

Confidence level: 7.81e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Acetamide, N-(3-(trifluoromethyl)phenyl)- (9CI)

Measured: 56.2

Predicted: 73.5

[Image not found](#)

3,4-Dichloroacetanilide

Measured: 219

Predicted: 111

[Image not found](#)

1-Naphthaleneacetic acid

Measured: 158

Predicted: 165

[Image not found](#)

MCPA

Measured: 53.7

Predicted: 74.5

[Image not found](#)

Acetamide, N-(3-chloro-4-methoxyphenyl)-

Measured: 89.1

Predicted: 99.8