

2-(Methylsulfanyl)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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 67.2 °C

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 7.50e-01

Nearest Neighbors from the Training Set

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N-Nitrosodiphenylamine

Measured: 66.5

Predicted: 61.8

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Pyridazine, 3-(2-methylphenoxy)-

Measured: 78.0

Predicted: 77.2

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Fenclorim [ISO]

Measured: 96.9

Predicted: 88.4