

Indoline, 1-(2-pyridylmethyl)-
20948-77-0 | DTXSID40175125

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
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.18 days

Global applicability domain: Outside

Local applicability domain index: 3.50e-01

Confidence level: 9.22e-01

Nearest Neighbors from the Training Set

Image not found

3-Methylindene

Measured: 12.5

Predicted: 2.76

Image not found

1H-Indene, 2-methyl-

Measured: 12.5

Predicted: 2.48

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 24.3

Predicted: 3.89

Image not found

2-Ethyl-p-xylene

Measured: 12.5

Predicted: 3.70

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1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17