

4-(1-Cyanoethyl)-1,2,3,4-tetrahydronaphthalene-1-carbonitrile
57964-39-3 | DTXSID2057576

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: 3.35 days

Global applicability domain: Outside

Local applicability domain index: 3.09e-01

Confidence level: 9.19e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5

Predicted: 3.17

Image not found

3-Ethyltoluene

Measured: 12.5

Predicted: 3.26

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 24.3

Predicted: 3.89

Image not found

1-Ethyl-2-methylbenzene

Measured: 24.3

Predicted: 3.88

Image not found

2-Ethyl-p-xylene

Measured: 12.5

Predicted: 3.70