

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 131 °C

Global applicability domain: Inside

Local applicability domain index: 4.82e-01

Confidence level: 4.30e-01

Nearest Neighbors from the Training Set

Image not found

[1,1'-Biphenyl]-4,4'-dicarbonitrile

Measured: 238

Predicted: 206

Image not found

Acetonitrile, m-phenylenedi-

Measured: 33.5

Predicted: 66.5

Image not found

Malononitrile, benzylidene-

Measured: 84.0

Predicted: 87.8

Image not found

1,3,4-Oxadiazole, 2-5-diphenyl-

Measured: 139

Predicted: 121

Image not found

3,5-Diphenyl-1,2,4-oxadiazole

Measured: 109

Predicted: 119