

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 750 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 4.98e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl 1-naphthaleneacetate

Measured: 302

Predicted: 425

[Image not found](#)

3,3'-Dichlorobenzidine

Measured: 22400

Predicted: 1680

[Image not found](#)

Carbofuran

Measured: 56.2

Predicted: 110

[Image not found](#)

Bendiocarb

Measured: 562

Predicted: 247

[Image not found](#)

2-Acetylaminofluorene

Measured: 1380

Predicted: 1860