

1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-  
59950-41-3 | DTXSID40208664

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
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** 2.69

**Global applicability domain:** Inside

**Local applicability domain index:** 4.45e-01

**Confidence level:** 6.87e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Aniline mustard

**Measured:** 2.90

**Predicted:** 3.02

[Image not found](#)

4-Chloro-5-(dimethylamino)-2-phenyl-3(2H)-pyridazinone

**Measured:** 1.55

**Predicted:** 1.91

[Image not found](#)

1-Methyl-4-(4-chlorophenyl)-1,2,3,6-tetrahydropyridine

**Measured:** 3.32

**Predicted:** 3.08