

2-(6,7,8,9-tetrahydro-5H-carbazol-3-yl)acetonitrile
57411-92-4 | DTXSID10306303

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 337 °C

Global applicability domain: Inside

Local applicability domain index: 3.31e-01

Confidence level: 5.42e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Nitrosodiphenylamine

Measured: 292

Predicted: 325

[Image not found](#)

4,4'-Methylenedianiline

Measured: 398

Predicted: 368

[Image not found](#)

1,2-Benzenediamine,N-phenyl-

Measured: 313

Predicted: 363

[Image not found](#)

N-Phenyl-1,4-benzenediamine

Measured: 354

Predicted: 363

[Image not found](#)

4,4'-Oxydianiline

Measured: 350

Predicted: 363