

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 156 °C

Global applicability domain: Inside

Local applicability domain index: 5.27e-01

Confidence level: 3.73e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Benzazol [INN:DCF]

Measured: 187

Predicted: 187

[Image not found](#)

2-Phenylbenzimidazole

Measured: 293

Predicted: 195

[Image not found](#)

4-cyanoquinoline

Measured: 104

Predicted: 89.8

[Image not found](#)

Quinoline-3-carbonitrile

Measured: 109

Predicted: 89.8