

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1330 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.13e-01

Confidence level: 6.68e-01

Nearest Neighbors from the Training Set

Image not found

2-Acetylaminofluorene

Measured: 1380

Predicted: 1860

Image not found

9-Anthracenecarboxylic acid

Measured: 550

Predicted: 1400

Image not found

9-Anthracenemethanol

Measured: 4070

Predicted: 5400

Image not found

Anthraquinone

Measured: 3720

Predicted: 2300

Image not found

Ethyl 1-naphthaleneacetate

Measured: 302

Predicted: 425