

2,3,4,9-tetrahydro-1h-carbazol-3-ylacetonitrile
40496-58-0 | DTXSID60300275

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.78e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.29e-01

Confidence level: 2.82e-01

Nearest Neighbors from the Training Set

Image not found

2,3-Benzofluorene

Measured: 1.35e-04

Predicted: 2.22e-07

Image not found

Tributyl phosphate

Measured: 2.09e-07

Predicted: 2.30e-03

Image not found

Clofentezine

Measured: 5.33e-11

Predicted: 1.59e-09

Image not found

Methyl salicylate

Measured: 5.27e-06

Predicted: 4.27e-03

Image not found

Flupoxam

Measured: 1.50e-07

Predicted: 5.80e-09