

N-Butyl-3-chloro-6-hydrazinylpyridazin-4-amine
61261-46-9 | DTXSID90615440

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: 5.94e-09 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.22e-01

Confidence level: 2.86e-01

Nearest Neighbors from the Training Set

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p,p'-DDE

Measured: 4.46e-11

Predicted: 2.89e-06

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Naphthalene, 1,2,4,7-tetrachloro-

Measured: 3.45e-10

Predicted: 1.23e-05

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Atrazine

Measured: 7.21e-11

Predicted: 2.03e-07

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1-Chlorotetradecane

Measured: 1.50e-07

Predicted: 1.27e-03

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Chloroneb

Measured: 5.53e-04

Predicted: 7.69e-03