

N-Butyl-6-chloro-3-hydrazinylpyridazin-4-amine
61261-44-7 | DTXSID70615443

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.47e-11 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.94e-01

Confidence level: 8.43e-01

Nearest Neighbors from the Training Set

Image not found

Dimethyl adipate

Measured: 8.40e-12

Predicted: 6.84e-12

Image not found

Bornyl acetate

Measured: 1.39e-11

Predicted: 1.36e-11

Image not found

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11

Image not found

Dimethyl glutarate

Measured: 3.30e-12

Predicted: 3.76e-12