

5,5-Bis[(²H₃)methyl]-3-[4-nitro-3-(trifluoromethyl)phenyl]imidazolidine-2,4-dione
1189477-66-4 | DTXSID60676068

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: 1.33e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.68e-01

Confidence level: 5.10e-01

Nearest Neighbors from the Training Set

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4-tert-Butylcyclohexyl acetate

Measured: 1.27e-05

Predicted: 2.32e-02

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Oxadiargyl

Measured: 3.00e-05

Predicted: 1.54e-08

Image not found

Sevoflurane

Measured: 2.48e-08

Predicted: 264

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2,2',3,4,4',5,5'-

Heptachlorobiphenyl

Measured: 3.75e-09

Predicted: 1.07e-06

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2,6-Dichlorodiphenyl ether

Measured: 3.60e-06

Predicted: 9.64e-04