

1-Dodecyl-2,4-dimethylpyridin-1-ium iodide
88477-51-4 | DTXSID00748410

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: 1.36e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.04e-01

Confidence level: 7.13e-01

Nearest Neighbors from the Training Set

Image not found

Quinoline, 2,4-dimethyl-

Measured: 2.38e-05

Predicted: 4.98e-03

Image not found

2-Phenoxyethanol

Measured: 1.27e-05

Predicted: 1.13e-02

Image not found

4,4'-Dichlorobiphenyl

Measured: 7.20e-06

Predicted: 1.18e-03

Image not found

Simazine

Measured: 5.11e-05

Predicted: 1.09e-07

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1-Nonanethiol

Measured: 3.56e-06

Predicted: 1.84e-01