

1,4-Diazabicyclo[2.2.2]octane
280-57-9 | DTXSID0022016

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: 6.27e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.97e-01

Confidence level: 5.52e-01

Nearest Neighbors from the Training Set

Image not found

Bicyclo(2.2.2)octane

Measured: 7.42e-01

Predicted: 2.31

Image not found

3-Bromothiophene

Measured: 3.45e-01

Predicted: 12.1

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1,2,3,4-Tetramethylbenzene

Measured: 1.25

Predicted: 8.44e-01

Image not found

Phenylhydrazine

Measured: 2.80e-02

Predicted: 8.40e-03

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2-Ethylpyridine

Measured: 1.91

Predicted: 5.66e-01