

Dipropylamine
142-84-7 | DTXSID2025185

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: 38.5 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.20e-01

Confidence level: 7.34e-01

Nearest Neighbors from the Training Set

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Tetrahydropyran

Measured: 20.1

Predicted: 81.9

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2-Pentanone

Measured: 79.4

Predicted: 28.9

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1,3,5-Trioxane

Measured: 32.1

Predicted: 10.4

Image not found

2-Methoxyethanol

Measured: 237

Predicted: 7.46

Image not found

Butyraldehyde

Measured: 62.7

Predicted: 101