

Butylamine
109-73-9 | DTXSID1021904

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: 107 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.31e-01

Confidence level: 8.10e-01

Nearest Neighbors from the Training Set

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5-Hexen-2-one

Measured: 92.9

Predicted: 11.2

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(2E)-1,4-Dichlorobut-2-ene

Measured: 30.0

Predicted: 7.15

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(2Z)-1,4-Dichlorobut-2-ene

Measured: 30.0

Predicted: 7.15

[Image not found](#)

Isoprene

Measured: 138

Predicted: 559

[Image not found](#)

1-Bromopropane

Measured: 310

Predicted: 115

[Image not found](#)

1,1'-Biphenyl,
2,2',3,3',4,4',5,5',6,6'-decabromo-

Measured: 178

Predicted: 1.49e-10