

4-Isobutylmorpholine
10315-98-7 | DTXSID30145675

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: 2.13 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Benzonitrile

Measured: 5.03

Predicted: 6.44e-01

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2-tert-Butyl-4-ethylphenol

Measured: 2.12

Predicted: 2.17e-02

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2-Ethoxyethanol

Measured: 5.40e-01

Predicted: 5.91

[Image not found](#)

Geraniol

Measured: 6.80e-01

Predicted: 3.39e-02

[Image not found](#)

(2Z)-3,7-Dimethylocta-2,6-dien-1-ol

Measured: 6.80e-01

Predicted: 3.39e-02

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3-Ethylphenol

Measured: 10.8

Predicted: 4.00e-02