

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.16

Global applicability domain: Inside

Local applicability domain index: 5.26e-01

Confidence level: 8.03e-01

Nearest Neighbors from the Training Set

[Image not found](#)

4-Isobutylmorpholine

Measured: 1.17

Predicted: 1.16

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Piperidine, 1-ethyl-

Measured: 1.75

Predicted: 1.58

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Nitrogen mustard

Measured: 0.91

Predicted: 1.07

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Quinuclidine

Measured: 1.38

Predicted: 1.35

[Image not found](#)

Diethylene glycol diethyl ether

Measured: 0.39

Predicted: 3.03e-01