

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	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.02e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.07e-01

Confidence level: 8.12e-01

Nearest Neighbors from the Training Set

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Butane, 1,1'-
[methylenebis(oxy)]bis-
Measured: 3.39e-11
Predicted: 3.22e-11

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1-Butoxy-2-propanol
Measured: 3.76e-11
Predicted: 3.73e-11

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Pentyl ether
Measured: 3.32e-11
Predicted: 2.70e-11

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1,8-Cineol
Measured: 1.11e-11
Predicted: 1.72e-11