

1-Nitrobutane

627-05-4 | DTXSID8020967

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: 6.23 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.32e-01

Confidence level: 8.27e-01

Nearest Neighbors from the Training Set

No Similar Structures Found.