

Propane, 2-methyl-2-nitro-
594-70-7 | DTXSID0060488

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 10.5

Global applicability domain: Inside

Local applicability domain index: 5.87e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

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1,2-Dibromoethane

Measured: 15.1

Predicted: 13.4

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2-Nitropropane

Measured: 8.32

Predicted: 7.41

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Isoprene

Measured: 20.0

Predicted: 15.6

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Thiophene, 3-methyl-

Measured: 5.25

Predicted: 7.49

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Thiophene

Measured: 8.91

Predicted: 6.68