

# 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
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** 1.35

**Global applicability domain:** Inside

**Local applicability domain index:** 7.59e-01

**Confidence level:** 8.91e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

1-Nitrobutane

**Measured:** 1.47

**Predicted:** 1.35

[Image not found](#)

Propane, 2-methyl-1-nitro-

**Measured:** 1.40

**Predicted:** 1.42

[Image not found](#)

2-Nitrobutane

**Measured:** 1.20

**Predicted:** 1.33

[Image not found](#)

2-Nitropropane

**Measured:** 0.93

**Predicted:** 1.03

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Propane, 2-methyl-2-nitro-

**Measured:** 1.17

**Predicted:** 1.33