

# Isopropanol

67-63-0 | DTXSID7020762

## Model Performance

Model

Data

### 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:** -11.2 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 7.36e-01

**Confidence level:** 6.66e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Isopropanol

**Measured:** -11.3

**Predicted:** -11.2

[Image not found](#)

1-Propanol

**Measured:** -11.3

**Predicted:** -11.1

[Image not found](#)

1,4-

Diazabicyclo[2.2.2]octane

**Measured:** -10.7

**Predicted:** -10.9

[Image not found](#)

Diethyl ether

**Measured:** -10.9

**Predicted:** -11.0

[Image not found](#)

tert-Butyl alcohol

**Measured:** -12.0

**Predicted:** -11.5