

# Propylene glycol diacetate

623-84-7 | DTXSID9044827

## 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:** -11.3 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 5.91e-01

**Confidence level:** 7.51e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Dimethyl glutarate

**Measured:** -11.5

**Predicted:** -11.4

[Image not found](#)

Dimethyl adipate

**Measured:** -11.1

**Predicted:** -11.2

[Image not found](#)

Dimethyl succinate

**Measured:** -11.9

**Predicted:** -11.7

[Image not found](#)

Ethyl 3-ethoxypropionate

**Measured:** -10.6

**Predicted:** -10.8

[Image not found](#)

2-Ethoxyethyl isobutyrate

**Measured:** -10.9

**Predicted:** -10.9