

Glycine ethyl ester  
459-73-4 | DTXSID90196648

### 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:**  $7.00 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $6.44 \times 10^{-1}$

**Confidence level:**  $8.06 \times 10^{-1}$

## Nearest Neighbors from the Training Set

Image not found

2-Ethoxyethyl acetate

**Measured:**  $1.30 \times 10^{-11}$

**Predicted:**  $1.03 \times 10^{-11}$

Image not found

Ethyl lactate

**Measured:**  $3.90 \times 10^{-12}$

**Predicted:**  $4.80 \times 10^{-12}$

Image not found

Methyl 2-hydroxypropanoate

**Measured:**  $2.80 \times 10^{-12}$

**Predicted:**  $3.16 \times 10^{-12}$

Image not found

Ethyl 3-ethoxypropionate

**Measured:**  $2.29 \times 10^{-11}$

**Predicted:**  $1.63 \times 10^{-11}$

Image not found

Butan-2-yl acetate

**Measured:**  $5.50 \times 10^{-12}$

**Predicted:**  $5.07 \times 10^{-12}$