

Pentyl acetate  
628-63-7 | DTXSID1027263

### 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	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:** 6.38e-12 cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:** 7.60e-01

**Confidence level:** 9.19e-01

## Nearest Neighbors from the Training Set

Image not found

Pentyl acetate

**Measured:** 7.55e-12

**Predicted:** 6.38e-12

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Butanoic acid, propyl ester

**Measured:** 7.41e-12

**Predicted:** 6.98e-12

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Butyl acetate

**Measured:** 4.90e-12

**Predicted:** 4.91e-12

Image not found

Propyl propionate

**Measured:** 4.02e-12

**Predicted:** 4.74e-12

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Ethyl butyrate

**Measured:** 4.94e-12

**Predicted:** 4.78e-12