

Ethyl hexanoate  
123-66-0 | DTXSID3021980

### 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
0.81	0.55	0.81	0.54	0.71	0.61

## Model Results

**Predicted value:** 110 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 6.26e-01

**Confidence level:** 7.62e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl hexanoate

**Measured:** 115

**Predicted:** 110

[Image not found](#)

1-Octanol

**Measured:** 36.3

**Predicted:** 42.5

[Image not found](#)

Ethyl valerate

**Measured:** 93.3

**Predicted:** 68.6

[Image not found](#)

Ethyl heptanoate

**Measured:** 407

**Predicted:** 284

[Image not found](#)

2-Phenylethyl acetate

**Measured:** 77.6

**Predicted:** 98.8