

Heptane  
142-82-5 | DTXSID6024127

### 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:** 322 L/kg

**Global applicability domain:** Inside

**Local applicability domain index:** 5.32e-01

**Confidence level:** 6.69e-01

## Nearest Neighbors from the Training Set

[Image not found](#)

Propylbenzene

**Measured:** 741

**Predicted:** 859

[Image not found](#)

Ethylbenzene

**Measured:** 170

**Predicted:** 271

[Image not found](#)

1-Heptanol

**Measured:** 13.8

**Predicted:** 18.6

[Image not found](#)

Styrene

**Measured:** 912

**Predicted:** 358

[Image not found](#)

Butylbenzene

**Measured:** 2450

**Predicted:** 1580