

Ethyl heptanoate
106-30-9 | DTXSID1040112

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 9.64e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.24e-01

Confidence level: 7.69e-01

Nearest Neighbors from the Training Set

Image not found

Geraniol

Measured: 6.80e-01

Predicted: 3.39e-02

Image not found

(2Z)-3,7-Dimethylocta-2,6-dien-1-ol

Measured: 6.80e-01

Predicted: 3.39e-02

Image not found

2-Ethoxyethanol

Measured: 5.40e-01

Predicted: 5.91

Image not found

Methyl valerate

Measured: 3.60

Predicted: 15.6

Image not found

4-Heptanol

Measured: 1.84

Predicted: 1.29

Image not found

Hexadecanoic acid, 1-methylethyl ester

Measured: 1.32

Predicted: 2.42e-05