

Ethyl heptanoate
106-30-9 | DTXSID1040112

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: 284 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.23e-01

Confidence level: 6.94e-01

Nearest Neighbors from the Training Set

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Ethyl heptanoate

Measured: 407

Predicted: 284

[Image not found](#)

1-Nonanol

Measured: 77.6

Predicted: 101

[Image not found](#)

Ethyl hexanoate

Measured: 115

Predicted: 110

[Image not found](#)

Ethyl octanoate

Measured: 1050

Predicted: 617

[Image not found](#)

Butanamide, N-phenyl-

Measured: 51.3

Predicted: 67.1