

Octaneperoxoic acid
33734-57-5 | DTXSID7074618

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: 112 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.58e-01

Confidence level: 8.02e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Ethyl heptanoate

Measured: 407

Predicted: 284

[Image not found](#)

Ethyl hexanoate

Measured: 115

Predicted: 110

[Image not found](#)

Carbamic acid, phenyl-, ethyl ester

Measured: 66.1

Predicted: 62.6

[Image not found](#)

Propham

Measured: 67.6

Predicted: 83.2

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Butanamide, N-phenyl-

Measured: 51.3

Predicted: 67.1