

Ethofumesate
26225-79-6 | DTXSID8034580

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.24e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.41e-01

Confidence level: 4.98e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Cyclobutanecarboxylic acid, 1-(phenylsulfonyl)-, methyl ester

Measured: 9.99e-04

Predicted: 1.53e-03

[Image not found](#)

Tetraethyl pyrophosphate

Measured: 3.45

Predicted: 3.46

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Phosphinic acid, dimorpholino-, phenyl ester

Measured: 2.47

Predicted: 1.62

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Cyclopropanecarboxylic acid, 1-(phenylsulfonyl)-, methyl ester

Measured: 5.49e-03

Predicted: 3.72e-03

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Cyclopentanecarboxylic acid, 1-(phenylsulfonyl)-, methyl ester

Measured: 2.82e-03

Predicted: 2.03e-03