

MLS000736649
6640-53-5 | DTXSID10287108

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: 4.43e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.07e-01

Confidence level: 5.48e-01

Nearest Neighbors from the Training Set

Image not found

4-Aminoacridine

Measured: 6.00e-05

Predicted: 1.96e-02

Image not found

N-(1-Naphthyl)ethylenediamine

Measured: 1.07e-02

Predicted: 9.11e-02

Image not found

1-(1-Naphthyl)-2-thiourea

Measured: 2.97e-03

Predicted: 1.77e-02

Image not found

1,10-Phenanthroline

Measured: 1.49e-02

Predicted: 5.60e-03

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Heptachlor epoxide

Measured: 5.14e-07

Predicted: 3.52e-07