

Deferoxamine
70-51-9 | DTXSID7022887

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: 21000 L/kg

Global applicability domain: Outside

Local applicability domain index: 9.66e-02

Confidence level: 6.15e-01

Nearest Neighbors from the Training Set

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Dioctyl phthalate

Measured: 24000

Predicted: 17100

Image not found

Di(2-ethylhexyl) adipate

Measured: 15500

Predicted: 14400

Image not found

Bis(2-ethylhexyl) terephthalate

Measured: 14500

Predicted: 12500

Image not found

Fluvalinate

Measured: 507000

Predicted: 293000

Image not found

tau-Fluvalinate

Measured: 507000

Predicted: 284000