

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 142 °C

Global applicability domain: Outside

Local applicability domain index: 1.78e-01

Confidence level: 6.31e-01

Nearest Neighbors from the Training Set

Image not found

Deferoxamine

Measured: 140

Predicted: 142

Image not found

Puromycin

Measured: 176

Predicted: 176

Image not found

Psicofuranine

Measured: 212

Predicted: 215

Image not found

Hexamethylmelamine

Measured: 137

Predicted: 141

Image not found

Mopidamol

Measured: 158

Predicted: 164