

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
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.46e-10 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 6.93e-02

Confidence level: 8.97e-01

Nearest Neighbors from the Training Set

Image not found

beta-Caryophyllene

Measured: 2.00e-10

Predicted: 1.99e-10

Image not found

alpha-Humulene

Measured: 2.90e-10

Predicted: 2.87e-10

Image not found

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-

Measured: 4.80e-11

Predicted: 4.73e-11

Image not found

Myrcene

Measured: 2.15e-10

Predicted: 2.05e-10