

Chlorpheniramine maleate
113-92-8 | DTXSID4020321

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: 2.33e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.64e-01

Confidence level: 4.54e-01

Nearest Neighbors from the Training Set

Image not found

Sparteine

Measured: 1.30e-02

Predicted: 8.29e-03

Image not found

Dieldrin

Measured: 5.80e-07

Predicted: 3.60e-07

Image not found

Endrin

Measured: 5.80e-07

Predicted: 3.60e-07

Image not found

Heptachlor epoxide

Measured: 5.14e-07

Predicted: 3.52e-07

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Bis(ethylxanthogen)

Measured: 1.14e-05

Predicted: 4.06e-05