

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 139 °C

Global applicability domain: Inside

Local applicability domain index: 5.92e-01

Confidence level: 5.03e-01

Nearest Neighbors from the Training Set

Image not found

Michler's ketone

Measured: 179

Predicted: 156

Image not found

2,5-Cyclohexadien-1-one, 4-[[4-(dimethylamino)phenyl]imino]-

Measured: 134

Predicted: 127

Image not found

Clomipramine

Measured: 190

Predicted: 163

Image not found

Thenalidine

Measured: 96.0

Predicted: 101

Image not found

Pyridazine, 3-(2-methylphenoxy)-

Measured: 78.0

Predicted: 77.2