

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
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.78

Global applicability domain: Inside

Local applicability domain index: 9.89e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

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2,3',4,4'-Tetrachlorobiphenyl

Measured: 9.02

Predicted: 8.77

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2,3,4',6-Tetrachlorobiphenyl

Measured: 8.41

Predicted: 8.77

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2,2',3,5'-tetrachlorobiphenyl

Measured: 8.36

Predicted: 8.53

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3,3',4,4'-Tetrachlorobinphenyl

Measured: 9.70

Predicted: 8.88

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2,2',4,5'-Tetrachlorobiphenyl

Measured: 8.39

Predicted: 8.52