

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 29.1

Global applicability domain: Inside

Local applicability domain index: 5.34e-01

Confidence level: 5.59e-01

Nearest Neighbors from the Training Set

Image not found

Molinate

Measured: 25.7

Predicted: 14.8

Image not found

Isoamyl ether

Measured: 170

Predicted: 137

Image not found

Menthol

Measured: 10.8

Predicted: 23.5

Image not found

(1R,2S,5R)-(-)-Menthol

Measured: 10.8

Predicted: 23.5

Image not found

N,N-Diethylaniline

Measured: 102

Predicted: 12.8