

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: 4.50

Global applicability domain: Inside

Local applicability domain index: 9.69e-01

Confidence level: 6.33e-01

Nearest Neighbors from the Training Set

Image not found

Hexyl acetate

Measured: 4.58

Predicted: 4.51

Image not found

Octanal

Measured: 5.36

Predicted: 4.54

Image not found

Propylbenzene

Measured: 4.09

Predicted: 4.53

Image not found

Cumene

Measured: 3.98

Predicted: 3.95

Image not found

Benzonitrile

Measured: 4.46

Predicted: 3.95