

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: 9.41

Global applicability domain: Inside

Local applicability domain index: 9.96e-01

Confidence level: 5.45e-01

Nearest Neighbors from the Training Set

Image not found

Aldrin

Measured: 8.08

Predicted: 9.41

Image not found

2,3,7,8-Tetrachlorodibenzofuran

Measured: 10.0

Predicted: 9.42

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1,2,7,8-Tetrachlorodibenzofuran

Measured: 9.78

Predicted: 9.42

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Naphthalene, 1,2,4,5,6,8-hexachloro-

Measured: 9.69

Predicted: 9.42

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2,4,4'-Tribromodiphenyl ether (BDE 28)

Measured: 9.50

Predicted: 9.41