

1-Dodecyl-2-methylpyridin-1-ium iodide
14402-22-3 | DTXSID60506018

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: 8.53

Global applicability domain: Inside

Local applicability domain index: 9.91e-01

Confidence level: 8.07e-01

Nearest Neighbors from the Training Set

Image not found

2,2',4,5'-Tetrachlorobiphenyl

Measured: 8.39

Predicted: 8.52

Image not found

2,2',5,6'-Tetrachlorobiphenyl

Measured: 8.45

Predicted: 8.52

Image not found

2,2',3,5'-tetrachlorobiphenyl

Measured: 8.36

Predicted: 8.53

Image not found

2,2',5,5'-Tetrachlorobiphenyl

Measured: 8.47

Predicted: 8.66

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2,3',4,4'-Tetrachlorobiphenyl

Measured: 9.02

Predicted: 8.77