

Fthalide
27355-22-2 | DTXSID2058045

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: 8.18

Global applicability domain: Inside

Local applicability domain index: 9.93e-01

Confidence level: 8.40e-01

Nearest Neighbors from the Training Set

Image not found

1,3,5,8-Tetrachloronaphthalene

Measured: 8.28

Predicted: 8.21

Image not found

1,3,5,7-Tetrachloronaphthalene

Measured: 7.90

Predicted: 8.21

Image not found

2,4,5-Trichlorobiphenyl

Measured: 8.00

Predicted: 8.15