

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
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1600 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.91e-01

Confidence level: 5.01e-01

Nearest Neighbors from the Training Set

Image not found

Fthalide

Measured: 2000

Predicted: 1600

Image not found

Chlorothalonil

Measured: 1820

Predicted: 1300

Image not found

Dichlone

Measured: 9550

Predicted: 3350

Image not found

Sulfone, methyl
pentafluorophenyl

Measured: 28.8

Predicted: 104

Image not found

Tetrachlorophthalic acid

Measured: 2000

Predicted: 1980