

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
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 13.9

Global applicability domain: Inside

Local applicability domain index: 3.85e-01

Confidence level: 6.29e-01

Nearest Neighbors from the Training Set

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1,1,1-Trichloro-2-methyl-2-propanol

Measured: 1.70

Predicted: 2.82

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Captan

Measured: 95.5

Predicted: 103

[Image not found](#)

Trichloroethylene

Measured: 15.8

Predicted: 15.2

[Image not found](#)

1-Chloro-4-nitrobenzene

Measured: 20.0

Predicted: 12.2

[Image not found](#)

bis(2-Chloro-1-methylethyl) ether

Measured: 12.0

Predicted: 9.79