

Sulfone, methyl pentafluorophenyl
651-85-4 | DTXSID30215403

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 62.4 °C

Global applicability domain: Inside

Local applicability domain index: 4.09e-01

Confidence level: 4.86e-01

Nearest Neighbors from the Training Set

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Transfluthrin

Measured: 32.0

Predicted: 40.0

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Tefluthrin

Measured: 44.6

Predicted: 42.9

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Chlorthal-dimethyl

Measured: 155

Predicted: 123

Image not found

Ethylene glycol

bis(trichloroacetate)

Measured: 40.0

Predicted: 47.4

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Erbon

Measured: 49.5

Predicted: 59.8