

Flucythrinate
70124-77-5 | DTXSID0022301

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 427 °C

Global applicability domain: Outside

Local applicability domain index: 2.23e-01

Confidence level: 4.52e-01

Nearest Neighbors from the Training Set

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Nonylphenyl diphenyl
phosphate, mixed isomers
Measured: 471
Predicted: 446

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Tetraphenoxysilane
Measured: 417
Predicted: 436

Image not found

Triphenyl phosphite
Measured: 360
Predicted: 403

Image not found

2-Ethylhexyl diphenyl phosphate
Measured: 375
Predicted: 369

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Octachlorodibenzo-p-dioxin
Measured: 510
Predicted: 400