

1,1,1,3,3-Pentafluoro-3-(1,2,2,2-tetrafluoroethoxy)propan-2-one
88457-11-8 | DTXSID00748238

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: 2.49

Global applicability domain: Outside

Local applicability domain index: 2.79e-01

Confidence level: 8.17e-01

Nearest Neighbors from the Training Set

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1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 2.51

Predicted: 2.40

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Triallyl phosphate

Measured: 1.20

Predicted: 1.41

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o-Toluenesulfonamide

Measured: 2.57

Predicted: 2.00

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Fenitrooxone

Measured: 2.75

Predicted: 1.68

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Benzenesulfonamide

Measured: 4.79

Predicted: 2.10