

1,1,1,3,3,3-Hexafluoropropan-2-yl trifluoroacetate
42031-15-2 | DTXSID80340673

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: 201 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.91e-01

Confidence level: 5.30e-01

Nearest Neighbors from the Training Set

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Benzoic acid, 3,6-dichloro-2-hydroxy-

Measured: 200

Predicted: 49.9

Image not found

Sulfone, methyl pentafluorophenyl

Measured: 28.8

Predicted: 104

Image not found

Dicloran

Measured: 1000

Predicted: 685

Image not found

Etridiazole

Measured: 1000

Predicted: 82.5

Image not found

Chlorfenac

Measured: 63.1

Predicted: 72.5