

Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-
163702-07-6 | DTXSID4073120

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: 404 L/kg

Global applicability domain: Outside

Local applicability domain index: 4.80e-01

Confidence level: 6.72e-01

Nearest Neighbors from the Training Set

Image not found

Dicloran

Measured: 1000

Predicted: 685

Image not found

3-Trifluoromethyl-4-nitrophenol

Measured: 129

Predicted: 219

Image not found

3,4,5-Trichloro-2-methoxyphenol

Measured: 631

Predicted: 102

Image not found

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

Measured: 200

Predicted: 49.9

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4,5,6-Trichloroguaiacol

Measured: 631

Predicted: 134