

1-Hexanol, 3,3,4,4,5,5,6,6,6-nonafluoro-
2043-47-2 | DTXSID1062122

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: 261 L/kg

Global applicability domain: Outside

Local applicability domain index: 4.66e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

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3-Trifluoromethyl-4-nitrophenol

Measured: 129

Predicted: 219

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Chlorfenac

Measured: 63.1

Predicted: 72.5

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2,3,6-Trichlorophenylacetic acid
sodium salt

Measured: 52.5

Predicted: 72.4

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Dicloran

Measured: 1000

Predicted: 685

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Pyroxychlor

Measured: 3020

Predicted: 161