

3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol
647-42-7 | DTXSID5044572

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: 3460 L/kg

Global applicability domain: Outside

Local applicability domain index: 3.48e-01

Confidence level: 6.44e-01

Nearest Neighbors from the Training Set

Image not found

Niclosamide

Measured: 2240

Predicted: 4670

Image not found

Nitrofen

Measured: 10000

Predicted: 3290

Image not found

Benzenamine, 2,6-dinitro-N-propyl-4-(trifluoromethyl)-

Measured: 4070

Predicted: 2330

Image not found

Benodanil

Measured: 661

Predicted: 828

Image not found

Chlornitrofen

Measured: 7940

Predicted: 25800