

Perfluoroheptanoic acid
375-85-9 | DTXSID1037303

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: 2110 L/kg

Global applicability domain: Outside

Local applicability domain index: 3.20e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

Image not found

Chlorthal-dimethyl

Measured: 5010

Predicted: 2160

Image not found

Benodanil

Measured: 661

Predicted: 828

Image not found

Fthalide

Measured: 2000

Predicted: 1600

Image not found

Tetrachlorovinphos

Measured: 1020

Predicted: 1070

Image not found

Z-Tetrachlorvinphos

Measured: 1020

Predicted: 1070

Image not found

Tridiphane

Measured: 5620

Predicted: 6630