

1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-
2706-91-4 | DTXSID8062600

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
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.18

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 4.02e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Pretilachlor

Measured: 4.08

Predicted: 3.75

[Image not found](#)

Venlafaxine hydrochloride

Measured: 0.43

Predicted: 2.49