

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

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 121 °C

Global applicability domain: Inside

Local applicability domain index: 2.63e-01

Confidence level: 5.58e-01

Nearest Neighbors from the Training Set

Image not found

1-Octanol,
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-
pentadecafluoro-
Measured: 161
Predicted: 156

Image not found

1-Pentanol, 2,2,3,3,4,4,5,5-
octafluoro-
Measured: 141
Predicted: 129

Image not found

2-Propanol, 1,1,1,3,3,3-
hexafluoro-2-(trifluoromethyl)-
Measured: 45.0
Predicted: 55.1

Image not found

1-Octene,
3,3,4,4,5,5,6,6,7,7,8,8,8-
tridecafluoro-
Measured: 104
Predicted: 101