

1-Hexadecanol
36653-82-4 | DTXSID4027991

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.39e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.87e-01

Confidence level: 7.36e-01

Nearest Neighbors from the Training Set

Image not found

1-Hexadecene

Measured: 3.85e-05

Predicted: 1.74e-03

Image not found

1-Dodecanol

Measured: 1.10e-04

Predicted: 9.62e-04

Image not found

1-Bromooctadecane

Measured: 2.70e-06

Predicted: 8.30e-06

Image not found

Methyl linoleate

Measured: 4.36e-04

Predicted: 4.52e-06