

2-hydroxy-2,4,4-trimethylpentanoic acid
5438-26-6 | DTXSID90280379

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: 6.07e-04 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.33e-01

Confidence level: 3.97e-01

Nearest Neighbors from the Training Set

Image not found

Pentan-2-ol

Measured: 3.14e-06

Predicted: 5.03

Image not found

2,4,4-Trimethyl-1-pentene

Measured: 1.30e-02

Predicted: 45.3

Image not found

Heptane

Measured: 4.50e-03

Predicted: 42.3

Image not found

Dicofol

Measured: 1.00e-04

Predicted: 2.79e-07

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Heptacosane

Measured: 8.75e-03

Predicted: 1.05e-07