

Isopentyl alcohol
123-51-3 | DTXSID3025469

Model Performance

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

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: 4.58 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.55e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Diacetone alcohol

Measured: 2.37

Predicted: 1.27

[Image not found](#)

Thiram

Measured: 3.12

Predicted: 1.60e-05

[Image not found](#)

Cyclohexane, tridecyl-

Measured: 6.11

Predicted: 9.77e-06

[Image not found](#)

Isobutylamine

Measured: 10.4

Predicted: 172

[Image not found](#)

2-Chloropropan-1-ol

Measured: 18.3

Predicted: 4.93