

1-Pentanol
71-41-0 | DTXSID6021741

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 130 °C

Global applicability domain: Inside

Local applicability domain index: 8.71e-01

Confidence level: 8.61e-01

Nearest Neighbors from the Training Set

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1-Pentanol

Measured: 138

Predicted: 130

[Image not found](#)

Isopentyl alcohol

Measured: 131

Predicted: 124

[Image not found](#)

2-Methyl-1-butanol

Measured: 128

Predicted: 123

[Image not found](#)

Pentan-2-ol

Measured: 119

Predicted: 121

[Image not found](#)

3-Pentanol

Measured: 116

Predicted: 119