

tert-Butyl alcohol
75-65-0 | DTXSID8020204

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
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.23 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.91e-01

Confidence level: 6.79e-01

Nearest Neighbors from the Training Set

[Image not found](#)

tert-Butyl alcohol

Measured: 13.5

Predicted: 5.23

[Image not found](#)

2-Butanol

Measured: 2.44

Predicted: 1.98

[Image not found](#)

2-Methyl-3-buten-2-ol

Measured: 11.6

Predicted: 5.01