

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 22.4 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.36e-01

Confidence level: 7.58e-01

Nearest Neighbors from the Training Set

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Bromotrifluoromethane

Measured: 40.7

Predicted: 6290

[Image not found](#)

Cyclobutane, methyl-

Measured: 9.15

Predicted: 594

[Image not found](#)

2,2-Dimethylbutane

Measured: 16.0

Predicted: 225

[Image not found](#)

2-Chloropropan-1-ol

Measured: 18.3

Predicted: 4.93

[Image not found](#)

Trichlorofluoromethane

Measured: 16.7

Predicted: 651