

tert-Butyl alcohol
75-65-0 | DTXSID8020204

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: -11.0 °C

Global applicability domain: Inside

Local applicability domain index: 8.04e-01

Confidence level: 4.01e-01

Nearest Neighbors from the Training Set

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tert-Butyl alcohol

Measured: 25.4

Predicted: -11.0

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Pentan-2-ol

Measured: -73.0

Predicted: -37.3

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2,2-Dimethylpropanol

Measured: 52.5

Predicted: -31.2

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2-Butanol

Measured: -115

Predicted: -70.5

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2-Methyl-3-buten-2-ol

Measured: -28.0

Predicted: -32.6