

1-Butanol, 3-methoxy-3-methyl-, acetate
103429-90-9 | DTXSID30145852

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: -54.9 °C

Global applicability domain: Inside

Local applicability domain index: 7.50e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

Image not found

2-Butoxyethyl acetate

Measured: -63.0

Predicted: -54.2

Image not found

2-Ethoxyethyl acetate

Measured: -61.7

Predicted: -56.7

Image not found

2-Ethoxyethyl acrylate

Measured: -47.0

Predicted: -54.7

Image not found

2-Methoxyethyl acetate

Measured: -70.0

Predicted: -63.1

Image not found

Propanedioic acid, bis(1,1-dimethylethyl) ester

Measured: -6.00

Predicted: -11.0