

Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-
163702-07-6 | DTXSID4073120

Model Performance

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

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 3.36

Global applicability domain: Inside

Local applicability domain index: 4.12e-01

Confidence level: 5.53e-01

Nearest Neighbors from the Training Set

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Perflenapent

Measured: 4.40

Predicted: 4.23

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1-Hexanol, 3,3,4,4,5,5,6,6,6-nonafluoro-

Measured: 3.30

Predicted: 3.01

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3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol

Measured: 4.54

Predicted: 4.45

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1-Butanol, 2,2,3,3,4,4,4-heptafluoro-

Measured: 1.94

Predicted: 1.93