

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

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
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -53.6 °C

Global applicability domain: Inside

Local applicability domain index: 4.48e-01

Confidence level: 5.25e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methyl heptafluorobutyrate

Measured: -86.0

Predicted: -70.3

[Image not found](#)

HCFC-226da

Measured: -120

Predicted: -109

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1,1,3,3,3-Pentafluoro-1,2,2-trichloropropane

Measured: -4.30

Predicted: -47.6