

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
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 55.8 °C

Global applicability domain: Inside

Local applicability domain index: 5.01e-01

Confidence level: 8.19e-01

Nearest Neighbors from the Training Set

Image not found

2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane

Measured: 42.1

Predicted: 39.1

Image not found

Sevoflurane

Measured: 58.5

Predicted: 55.0

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Cyclohexane, undecafluoro-

Measured: 62.0

Predicted: 58.2

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HFE-347pcf2

Measured: 56.2

Predicted: 56.2