

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
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 348 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.44e-01

Confidence level: 8.12e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Thiobencarb

Measured: 193

Predicted: 1.60e-05

[Image not found](#)

Fenfuram

Measured: 387

Predicted: 1.44e-06

[Image not found](#)

Benzene, 1-fluoro-2-(trifluoromethyl)-

Measured: 213

Predicted: 23.4

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Mepronil

Measured: 664

Predicted: 3.04e-07