

Chemical Name TRIFLUOROMETHOXYDIFLUOROAMINE

Molecular Formula (C F5.0 N O )

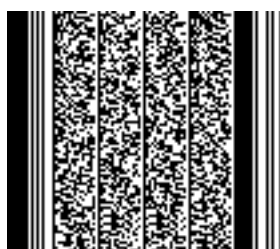
Difference Enthalpy-Energy(DIFF)-1.48(Ref.528)

Enthalpy of Formation(ENTH)-189.1(Ref.39)

Classification N.A

Oxygen Balance 17.52

Molecular Weight 137.009



# Opt=(Tight GDIIIS) B3LYP/6-31G(d) SCRF

FN(F)OC(F)(F)F

0 1

N 1.4019614542353322 -0.12231928581237403 0.016748849554652438

F 1.788113127358512 -1.3149781305410908 0.3839511527847748

F 2.2705741492912574 0.7055961273556137 0.5280421318778641

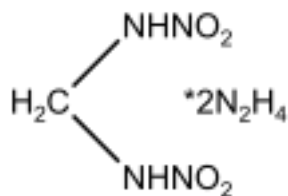
O 0.21430939901376292 0.15422521918347318 0.6255284917840827

C -0.9162511484990264 -0.15074010869476687 -0.207702643983676

F -1.0192674307652787 -1.4950889688575177 -0.47384349511000884

F -2.0434172153651082 0.22917376991038774 0.4733297065857297

F -0.8849191801064943 0.552926038947007 -1.3891535642716308



Chemical Name DIHYDRAZINE-METHYLENEDINITRAMINE SALT

Molecular Formula (C H12.0 N8.0 O4.0 )

Density(DICH)1.4(Ref.41)

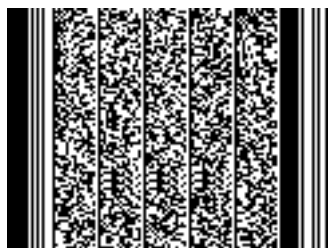
Difference Enthalpy-Energy(DIFF)-7.1(Ref.528)

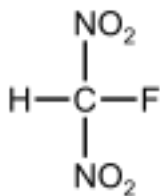
Enthalpy of Formation(ENTH)-10.8(Ref.41)

Classification N.A

Oxygen Balance -31.97

Molecular Weight 200.157





Chemical Name FLUORODINITROMETHANE

Molecular Formula (C F H N2.0 O4.0 )

Density(DICH)1.595(Ref.239)

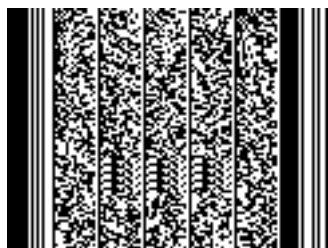
Difference Enthalpy-Energy(DIFF)-2.37(Ref.528)

Enthalpy of Formation(ENTH)-66.5(Ref.49)

Classification N.A

Oxygen Balance 25.8

Molecular Weight 124.028



# Opt=(Tight GDIIIS) B3LYP/6-31G(d) SCRF

[O-][N+](=O)C(F)[N+](O-)=O

0 1

C 0.2929918188520238 0.5041318214051043 0.4341780373426154

N 0.96430704744923 -0.14740381888590978 -0.6056323430744609

O 1.4901242009141928 0.4477825140176748 -1.4617968109073545

O 1.0215424346290674 -1.415714223208706 -0.6554348730571862

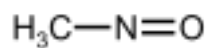
N -0.7738834891296269 1.2721095151784936 -0.04721939982275802

O -1.8407888333339975 0.8113288299662913 -0.16645553050955358

O -0.6157925571771365 2.4781216081877497 -0.4145472002658019

F 1.1851905279462265 1.276075665529946 1.1480383236717262

H -0.12370551798555157 -0.24125529806510015 1.1115711075761276



Chemical Name NITROSOMETHANE

Molecular Formula (C H3.0 N O )

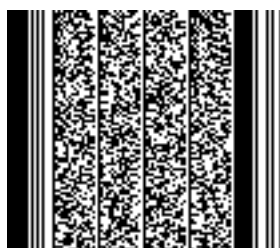
Difference Enthalpy-Energy(DIFF)-0.89(Ref.528)

Enthalpy of Formation(ENTH)16.7(Ref.49)

Classification N.A

Oxygen Balance -88.8

Molecular Weight 45.041



# Opt=(Tight GDIIS) B3LYP/6-31G(d) SCRF

CN=O

O 1

C 1.4020600574603024 -0.1690862189243901 -0.19283329291264384

N 0.03194130740113851 -0.02577939770140926 -0.07185556818357665

O -0.47578062392485576 1.0185566013184348 0.05232303825244582

H 1.8514503592810696 -0.21608995173192172 0.7991037039433045

H 1.6247478223270784 -1.087214352297816 -0.7364792163654629

H 1.8099119386598457 0.6830909650667827 -0.7364792163654629

