

Chemical Name METHANOL

Molecular Formula (C H4.0 O)

Density(DICH)0.791(Ref.H)

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

Enthalpy of Formation(ENTH)-57.01(Ref.C)

Enthalpy of Formation(ENTH)-57.02(Ref.ST)

Melting Point(SCHM)-97.7(Ref.135)

Boiling Point(SIED)64.5(Ref.135)

Heat of Combustion(VBW)173.45(Ref.C)

Classification Solvents(S)

Oxygen Balance -149.8

Molecular Weight 32.042



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

CO

0 1

C 1.4100156155263794 0.0012955465678606932 0.0022439686215908763

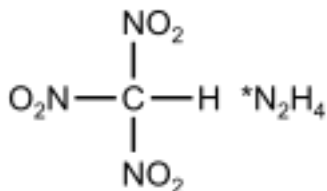
O -0.011101468291854764 -0.009706255201567902 -0.016811727124996786

H 1.759527597355242 0.004001348632944514 1.0346847917166706

H 1.7870840327822355 -0.8857932614330207 -0.5066694379887473

H 1.7733045852534481 0.8941159479067334 -0.5066694379887473

H -0.3431977008458324 -0.01227723050018041 0.8839132488856989



Chemical Name HYDRAZINIUM NITROFORMATE

Molecular Formula (C H5.0 N5.0 O6.0)

Density(DICH)1.91(Ref.322)

Density(DICH)1.87(Ref.1003)

Difference Enthalpy-Energy(DIFF)-4.74(Ref.528)

Enthalpy of Formation(ENTH)-18.37(Ref.525)

Enthalpy of Formation(ENTH)-17.2(Ref.278)

Enthalpy of Formation(ENTH)-17.2(Ref.SA)

Enthalpy of Formation(ENTH)-16.52(Ref.531)

Enthalpy of Formation(ENTH)-11.0(Ref.1410)

Melting Point(SCHM)118-124(*) (Ref.407)

Heat of Combustion(VBW)248.33(Ref.531)

Classification Energetic fillers(E)

Oxygen Balance 13.11

Molecular Weight 183.081



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

N[NH3+].[O-]C(=O)[N+](=[O-])=O

0 1

C -1.601895567655369 0.10065459354127182 -0.026154089846206596

O -0.757431071278917 -0.4499609436001194 0.7183206248979939

O -1.1357479419065029 0.9705299505503732 -0.9534153027740089

N -2.899866817416933 -0.1485139633585758 0.0784721876756076

O -3.326117586827541 -0.8943340233483403 0.8698193367094058

O -3.7355294925426312 0.42162438621539 -0.6870427566627912

N 2.9397059397780745 -0.0069880910273658016 0.012103728042353793

N 1.5458235527645567 0.006988091027365801 -0.012103728042353793

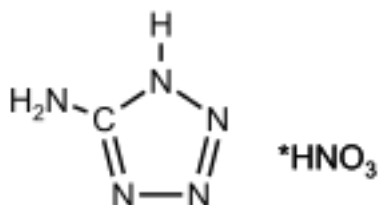
H 3.259771653020407 -0.010197326411519466 0.9700429954361308

H 3.27630326962743 -0.8350660857408471 -0.458097369584591

H 3.29283987370194 0.8141741051932537 -0.458097369584591

H 1.0496949229159422 0.8866923000770479 -0.020872264112297485

H 1.0321552055976178 -0.8625910841453008 -0.020872264112297485



Chemical Name 5-AMINOTETRAZOLE NITRATE

Molecular Formula (C H4.0 N6.0 O3.0)

Density(DICH)1.8(Ref.419)

Difference Enthalpy-Energy(DIFF)-3.85(Ref.528)

Enthalpy of Formation(ENTH)-6.59(Ref.C)

Enthalpy of Formation(ENTH)-6.6(Ref.SE)

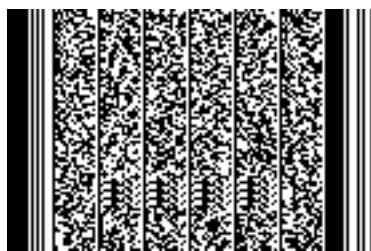
Melting Point(SCHM)160.0(Ref.419)

Heat of Combustion(VBW)224.09(Ref.C)

Classification N.A

Oxygen Balance -10.8

Molecular Weight 148.081



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

[O-][N+](O)=O.NC1=NN=NN1

-1 1

N -3.809536308612443 -0.2598248293222898 0.029701343761524272

N -3.205930780476553 -1.397913188461409 0.07487417431009444

N -1.9297558252823916 -1.172033817682502 0.04197743799790275

N -1.6970423300524544 0.10120439485591226 -0.025240762469417567

C -2.8901760104349563 0.7033244011369575 -0.03477788928791129

N -3.1190169819811873 2.025243039473331 -0.08653430431219258

N 2.7627430394733308 -0.021650635094611015 0.0

O 2.1802430394733303 -1.030570230503482 0.0

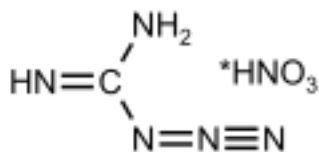
O 2.1302430394733314 1.073871500692704 0.0

O 4.0277430394733305 -0.021650635094611015 0.0

H -4.812858732645117 -0.1445757885278992 0.04242030713013037

H -2.343226918372703 2.671672295816032 -0.10600206613952942

H -4.066960450276157 2.3732720428140555 -0.10600206613952942



Chemical Name GUANYL AZIDE NITRATE

Molecular Formula (C H4.0 N6.0 O3.0)

Difference Enthalpy-Energy(DIFF)-3.85(Ref.528)

Enthalpy of Formation(ENTH)3.8(Ref.SE)

Enthalpy of Formation(ENTH)3.79(Ref.C)

Enthalpy of Formation(ENTH)4.69(Ref.230)

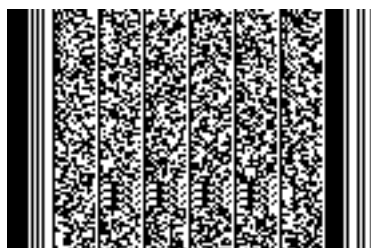
Heat of Combustion(VBW)234.47(Ref.C)

Density(DICH)1.5(Ref.999)

Classification Oxidizers(O)

Oxygen Balance -10.8

Molecular Weight 148.081



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

[N-]=[N+]=[N-]

-1 1

N 1.1610000000000003 0.0 0.0

N 0.0 0.0 0.0

N -1.1610000000000003 0.0 0.0

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

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

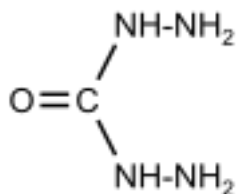
-1 1

N 0.0 0.0 0.0

O -0.5825000000000004 -1.008919595408871 0.0

O -0.6324999999999995 1.095522135787315 0.0

O 1.265 0.0 0.0



Chemical Name CARBOHYDRAZIDE

Molecular Formula (C H6.0 N4.0 O)

Density(DICH)1.616(Ref.B033)

Difference Enthalpy-Energy(DIFF)-3.26(Ref.528)

Enthalpy of Formation(ENTH)-27.96(Ref.10)

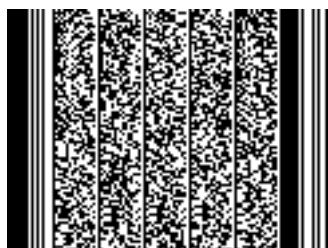
Melting Point(SCHM)154.0(Ref.H)

Heat of Combustion(VBW)271.6(Ref.10)

Classification N.A

Oxygen Balance -71.04

Molecular Weight 90.085



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

NNC(=O)NN

0 1

N 2.4104871152348206 -2.7797385930760097 2.1127329020709458

N 1.5129192095619348 -2.073105156587446 1.3970993991297638

C 1.7199971394965579 -0.7903393294801361 1.025599155731012

O 2.7616989568030004 -0.17429496782337447 1.3577904901649178

N 0.7596012318959519 -0.19868812691526438 0.2821493302311701

N 0.8382271316380804 1.0852548883124988 -0.1230010847380559

H 2.205680516474625 -3.7317247525039114 2.3808310358988285

H 3.287806332551053 -2.357205302593899 2.3808310358988285

H 0.6497252951754293 -2.523307345771049 1.1281862997456065

H -0.05166169063591719 -0.739226039802902 0.01800687764899317

H 1.7407188200254033 1.5125641578058466 -0.27470982079785056

H -0.005381557099107814 1.6194915771408323 -0.27470982079785056

