

Chemical Name 5-AMINO-1H-TETRAZOLE

Molecular Formula (C H3.0 N5.0)

Density(DICH)1.65(Ref.358)

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

Enthalpy of Formation(ENTH)49.66(Ref.C)

Enthalpy of Formation(ENTH)50.0(Ref.266)

Enthalpy of Formation(ENTH)49.67(Ref.765)

Melting Point(SCHM)209-210(*) (Ref.90)

Heat of Combustion(VBW)246.18(Ref.C)

Classification N.A

Oxygen Balance -65.83

Molecular Weight 85.068



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

NC1=NN=NN1

0 1

N -0.5287844426017433 1.0372358402210073 0.005016352181154501

N 0.07482108553414707 -0.10085251891811205 0.05018918272972467

N 1.3509960407283084 0.12502685186079512 0.01729244641753298

N 1.5837095359582456 1.3982650643992094 -0.04992575404978734

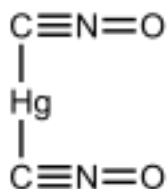
C 0.39057585557574365 2.0003850706802546 -0.05946288086828106

N 0.16173488402951267 3.322303709016628 -0.11121929589256235

H -1.5321068666344173 1.1524848810153978 0.017735315549760593

H 0.9375249476379971 3.968732965359329 -0.1306870577198992

H -0.786208584265457 3.6703327123573524 -0.1306870577198992



Chemical Name MERCURY FULMINATE

Molecular Formula (C2.0 Hg N2.0 O2.0)

Density(DICH)4.42(Ref.EX)

Difference Enthalpy-Energy(DIFF)-1.18(Ref.528)

Enthalpy of Formation(ENTH)64.05(Ref.SE)

Enthalpy of Formation(ENTH)64.1(Ref.ME)

Enthalpy of Formation(ENTH)65.4(Ref.192)

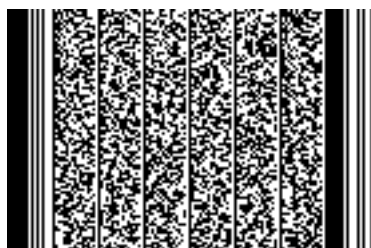
Heat of Combustion(VBW)267.0(Ref.27)

Melting Point(SCHM)160.0(Ref.325)

Classification Primary explosives(PX)

Oxygen Balance -16.86

Molecular Weight 284.624



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

[O-][N+]#C[Hg]C#[N+][O-]

0 1

O 1.3511773480469085 1.2153533998908714 0.0

N 0.34607157256850324 0.5486266611094179 0.0

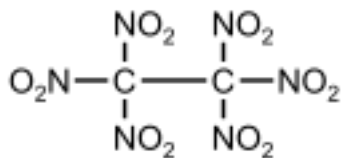
C -0.6084133041213635 -0.08949487834326095 0.0

Hg -2.348552407170017 -1.260712921025598 0.0

C -4.032919113515015 -2.510713202596308 0.0

N -4.952358820136058 -3.1983876024840905 0.0

O -5.916338506917695 -3.9234583012346174 0.0



Chemical Name HEXANITROETHANE

Molecular Formula (C2.0 N6.0 O12.0)

Density(DICH)1.85(Ref.807)

Density(DICH)1.998(Ref.585)

Density(DICH)1.05(Ref.EX)

Difference Enthalpy-Energy(DIFF)-5.33(Ref.528)

Enthalpy of Formation(ENTH)19.0(Ref.1431)

Enthalpy of Formation(ENTH)28.6(Ref.SE)

Enthalpy of Formation(ENTH)20.0(Ref.49)

Enthalpy of Formation(ENTH)20.4(Ref.91)

Melting Point(SCHM)150.0(Ref.148)

Heat of Combustion(VBW)207.1(Ref.1431)

Enthalpy of Formation(ENTH)28.6(Ref.STB)

Classification Oxidizers(O)

Oxygen Balance 42.66

Molecular Weight 300.055



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

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

0 1

C -0.8112732997790182 -1.4019709571947454 -2.9050681744280955

C 0.43790572825390245 -1.5535316419201617 -1.8828550887817783

N 1.2621289960794806 -0.38510263280261026 -1.7813210674380573

O 1.22831898397134 0.5257341596017665 -2.5111086717827833

O 2.1152539533857886 -0.2503846041780644 -0.844543663783541

N 1.3505253037029614 -2.5994975989190547 -2.2310369541215103

O 1.2880205085440326 -3.2502987967803674 -3.1983264500191093

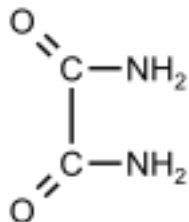
O 2.317699551812532 -2.9237169583469997 -1.4668566272050687

N -0.09240885756137104 -1.838368697974265 -0.5851392097501931

O -0.4681645570824622 -0.9992363054472304 0.13885086513408915

O -0.24033504447815615 -3.021486732707384 -0.1382609021554773

N -1.7671639541215938 -0.48610427912028453 -2.3543917410439326
O -1.4998746781846488 0.6265373808992053 -2.114878688560369
O -2.9785293388724376 -0.7878458067833822 -2.105624084023195
N -0.43429597278606025 -0.8895667512947577 -4.188273377305485
O -1.1970025256992625 -0.3598046677452976 -4.9004422469355715
O 0.7136169947264984 -1.0696034031565553 -4.702851884781366
N -1.4217971833596994 -2.6842521714359338 -3.1200067493916435
O -1.9549316013638143 -3.284801224097195 -2.2711426007072624
O -1.3973734401243265 -3.299568643834688 -4.2358626334588685



Chemical Name OXALIC ACID DIAMIDE

Molecular Formula (C2.0 H4.0 N2.0 O2.0)

Density(DICH)1.667(Ref.RP)

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

Enthalpy of Formation(ENTH)-120.6(Ref.925)

Enthalpy of Formation(ENTH)-121.2(Ref.STC)

Enthalpy of Formation(ENTH)-123.0(Ref.SE)

Enthalpy of Formation(ENTH)-119.3(Ref.99)

Enthalpy of Formation(ENTH)-123.2(Ref.C)

Enthalpy of Formation(ENTH)-109.2(Ref.926)

Melting Point(SCHM)350.0(Ref.RP)

Heat of Combustion(VBW)201.5(Ref.C)

Classification Coolants(CO)

Oxygen Balance -72.67

Molecular Weight 88.066



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

NC(=O)C(N)=O

0 1

C -1.2083069900046146 1.0326240373823994 -0.01133552471416529

O -2.436094387931727 1.2439448207626456 0.11774857398349195

C -0.6959269687754001 -0.27886239386611134 0.004193874691208729

O 0.5392968387182189 -0.48388723948102264 0.015173864461411772

N -0.4050241847506071 2.102513769203523 -0.17842347802194677

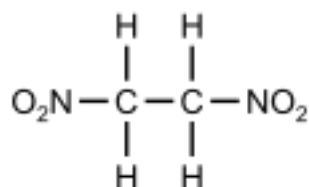
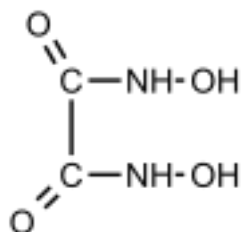
N -1.5069350885677437 -1.3536093520570582 -0.003023801157563231

H 0.5953243390000247 1.9780703294561697 -0.24100671326732648

H -0.8036293060049817 3.028417271722013 -0.24100671326732648

H -2.5093197360020856 -1.2298446957584928 -0.005730910174251859

H -1.1129145294350655 -2.2835773464211346 -0.005730910174251859



Chemical Name 1,2-DINITROETHANE

Molecular Formula (C2.0 H4.0 N2.0 O4.0)

Density(DICH)1.46(Ref.DL)

Difference Enthalpy-Energy(DIFF)-2.96(Ref.528)

Enthalpy of Formation(ENTH)-42.7(Ref.1431)

Enthalpy of Formation(ENTH)-43.9(Ref.STB)

Enthalpy of Formation(ENTH)-42.0(Ref.C)

Melting Point(SCHM)39.0(Ref.60)

Heat of Combustion(VBW)282.0(Ref.1431)

Classification N.A

Oxygen Balance -26.65

Molecular Weight 120.065



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

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

0 1

C -0.2180829684141754 -0.04029404107813525 -0.3443331785638602

C -0.4611234089892891 -1.3962010364656474 0.37171283077600764

N -0.7773045173068811 1.0238883602239126 0.36890492072472775

O -0.16723563230608282 1.6050251220543945 1.177931455884263

O -1.9804831053800314 1.3821872984578065 0.17001087191473124

N 0.09463199294251856 -2.4716387991745425 -0.32687286292709705

O 0.9261628304505688 -3.1462177067857837 0.14131722477167857

O -0.31092306799929154 -2.767648660124924 -1.4939480351528083
H 0.8530686613473761 0.16138997845615877 -0.336734341569787
H -0.7639690004892747 -0.05097699701500506 -1.2877282784227448
H 0.08219684709612596 -1.3816475400106736 1.3165362508224276
H -1.5325773980184971 -1.5961902286868468 0.36219062577346345