

Chemical Name SEMICARBAZIDE

Molecular Formula (C H5.0 N3.0 O)

Difference Enthalpy-Energy(DIFF)-2.66(Ref.622)

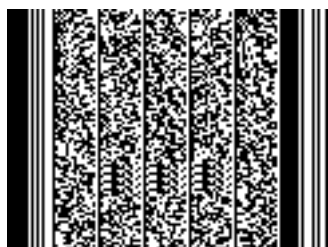
Enthalpy of Formation(ENTH)-53.94(Ref.622)

Heat of Combustion(VBW)210.9(Ref.622)

Classification N.A

Oxygen Balance -74.59

Molecular Weight 75.07



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

NNC(N)=O

0 1

N 0.9082578204929963 0.8064627381149918 -0.23990302431139834

N 0.9595809915587422 -0.4657497839374837 0.1958995452741486

C 1.7449964961306885 -0.8458401651119087 1.225571887340624

N 1.7970926896803605 -2.14180605122445 1.5690077894737946

O 2.4327663998069013 -0.02629447012519441 1.8768745264620723

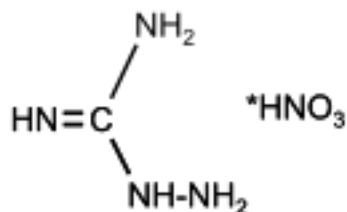
H 1.762973504009623 1.319119779642068 -0.40343851930686203

H 0.015023960303131467 1.2486045851357206 -0.40343851930686203

H 0.388817756052937 -1.1593825823647692 -0.26583941771346603

H 0.9427211178987844 -2.6647209679581336 1.6982718880815828

H 2.6906807059761384 -2.594455197853152 1.6982718880815828



Chemical Name AMINOGUANIDINE NITRATE

Molecular Formula (C H7.0 N5.0 O3.0)

Difference Enthalpy-Energy(DIFF)-4.44(Ref.528)

Enthalpy of Formation(ENTH)-66.62(Ref.525)

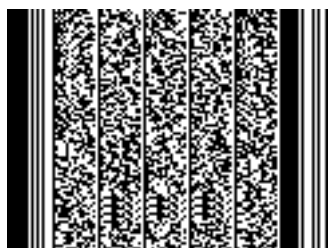
Melting Point(SCHM)144-146(*) (Ref.852)

Heat of Combustion(VBW)226.53(Ref.525)

Classification N.A

Oxygen Balance -29.18

Molecular Weight 137.098



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

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

-1 1

N -1.3688358089659718 0.9430196417114178 0.3052488719041837

C -2.5570618980426416 0.4007670351192749 0.11393415260171791

N -3.6153943774406185 1.1471500524131857 0.3206044676459452

N -2.7468615644264016 -0.8123901051003115 -0.25705941395494897

N -1.8545794718422013 -1.678546624143567 -0.4827280781968977

N 2.4160466241435667 -0.021650635094611015 0.0

O 1.8335466241435665 -1.030570230503482 0.0

O 1.7835466241435673 1.073871500692704 0.0

O 3.681046624143567 -0.021650635094611015 0.0

H -0.5511247358654745 0.35472392723553514 0.37843871585909356

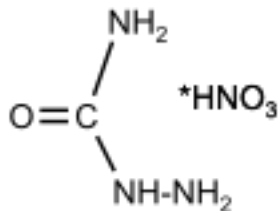
H -1.2774053130355765 1.9462064195129287 0.37843871585909356

H -3.5188182610678385 2.1493673702896605 0.40018776674089784

H -4.527042462245902 0.7197576472677244 0.40018776674089784

H -2.1072880862199517 -2.65225477294842 -0.5728990112646173

H -0.888808553327511 -1.3970226717327847 -0.5728990112646173



Chemical Name SEMICARBAZIDE NITRATE

Molecular Formula (C H6.0 N4.0 O4.0)

Density(DICH)1.75(Ref.952)

Difference Enthalpy-Energy(DIFF)-4.14(Ref.528)

Enthalpy of Formation(ENTH)-114.24(Ref.952)

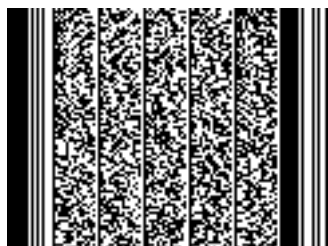
Melting Point(SCHM)115-119(*) (Ref.97)

Heat of Combustion(VBW)235.2(Ref.ICT)

Classification N.A

Oxygen Balance -11.59

Molecular Weight 138.083



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

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

-1 1

N -3.0174415638085827 1.3411082845718008 -1.1653931691592467

N -2.9661183927428367 0.06889576251932528 -0.7295905995736998

C -2.1807028881708903 -0.3111946186550998 0.30008174249277575

N -2.1286066946212183 -1.607160504767641 0.6435176446259463

O -1.4929329844946775 0.5083510763316146 0.951384381614224

N 2.3446605047676408 -0.021650635094611015 0.0

O 1.7621605047676405 -1.030570230503482 0.0

O 1.7121605047676414 1.073871500692704 0.0

O 3.609660504767641 -0.021650635094611015 0.0

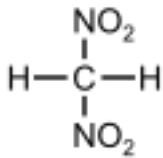
H -2.1627258802919562 1.853765326098877 -1.3289286641547104

H -3.910675423998448 1.7832501315925295 -1.3289286641547104

H -3.5368816282486417 -0.6247370359079601 -1.1913295625613145

H -2.982978266402794 -2.1300754215013247 0.7727817432337345

H -1.2350186783254402 -2.059809651396343 0.7727817432337345



Chemical Name DINITROMETHANE

Molecular Formula (C H2.0 N2.0 O4.0)

Density(DICH)1.524(Ref.12)

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

Enthalpy of Formation(ENTH)-25.2(Ref.12)

Melting Point(SCHM)< -15(*) (Ref.H)

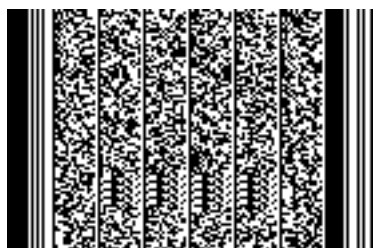
Boiling Point(SIED)100.0(Ref.H)

Heat of Combustion(VBW)137.3(Ref.12)

Classification N.A

Oxygen Balance 15.09

Molecular Weight 106.038



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

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

0 1

C -0.05441640615070148 -0.08293554793053222 -0.026032607590242764

N -0.8273834270756054 1.0321366033626527 0.30905043002273114

O -1.1607442062158233 1.804523008997037 -0.5007282065574744

O -1.162802173577957 1.2546593809841025 1.51257170654671

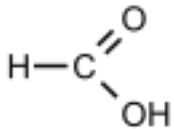
N 1.3115926194215468 0.19612860409206273 0.03833591642193679

O 1.8144625306238318 0.5128577153135324 1.0444644074221776

O 2.054784468358084 0.111128416715328 -0.9889041326189849

H -0.24937604545866396 -0.8323104653480631 0.7411231602863848

H -0.27202628468504453 -0.3034382074099 -1.071080222738373



Chemical Name FORMIC ACID

Molecular Formula (C H2.0 O2.0)

Density(DICH)1.22(Ref.H)

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

Enthalpy of Formation(ENTH)-101.52(Ref.ST)

Enthalpy of Formation(ENTH)-101.6(Ref.C)

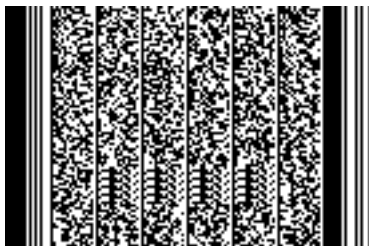
Melting Point(SCHM)8.0(Ref.RP)

Boiling Point(SIED)101.0(Ref.RP)

Classification N.A

Oxygen Balance -34.76

Molecular Weight 46.026



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

OC=O

0 1

C 1.354595592940829 -0.2422940535901912 -0.24577953652121048

O 1.8007013361584494 0.2233570085786851 -1.317017888950878

O 0.14218317077377288 0.1436063847129854 0.2054819965196633

H 1.9958373943746022 -0.9548683181456514 0.2730141311225021

H 0.14309001722019551 0.1433177432946447 1.1654815248089505