

Chemical Name SEMICARBAZIDE

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

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

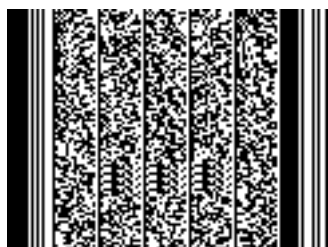
Enthalpy of Formation(ENTH)-53.94(Ref.622)

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

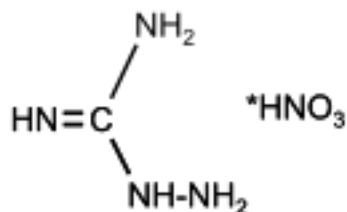
H 1.762973504009623 1.319119779642068 -0.40343851930686203

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)

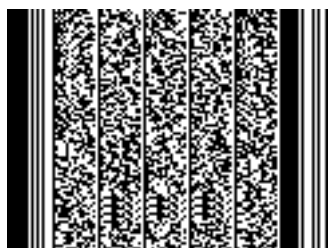
Melting Point(SCHM)144-146(*) (Ref.852)

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