

Chemical Name NITROGLYKOL

Molecular Formula (C2.0 H4.0 N2.0 O6.0)

Density(DICH)1.492(Ref.H)

Difference Enthalpy-Energy(DIFF)-3.55(Ref.528)

Enthalpy of Formation(ENTH)-58.02(Ref.C)

Enthalpy of Formation(ENTH)-58.24(Ref.9)

Enthalpy of Formation(ENTH)-54.39(Ref.102)

Enthalpy of Formation(ENTH)-67.7(Ref.549)

Enthalpy of Formation(ENTH)-59.6(Ref.549)

Melting Point(SCHM)-22.8(Ref.320)

Boiling Point(SIED)199.0(Ref.320)

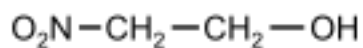
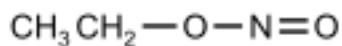
Heat of Combustion(VBW)268.2(Ref.ME)

Classification Plasticizers (Energetic)(PE)

Oxygen Balance 0.0

Molecular Weight 152.064





Chemical Name 2-NITROETHANOL

Molecular Formula (C2.0 H5.0 N O3.0)

Density(DICH)1.27(Ref.H)

Difference Enthalpy-Energy(DIFF)-2.66(Ref.528)

Enthalpy of Formation(ENTH)-83.6(Ref.STB)

Enthalpy of Formation(ENTH)-83.83(Ref.C)

Melting Point(SCHM)-80.0(Ref.H)

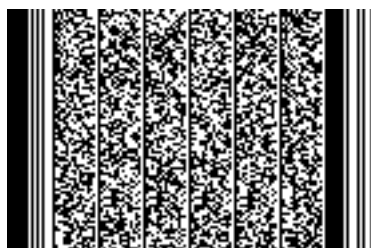
Boiling Point(SIED)194.0(Ref.H)

Heat of Combustion(VBW)275.06(Ref.C)

Classification N.A

Oxygen Balance -61.49

Molecular Weight 91.067



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

OCC[N+](O)=O

0 1

C -0.4573800153984795 0.439422231460497 0.4932542685295179

C -0.03564186554515802 0.5792309120578124 -0.9883914402689875

O -0.6488664085471363 -0.9291872900921193 0.8307038635661743

N 0.16784703451227684 1.912565882535228 -1.3523565636751451

O 1.2062754539022207 2.2949584283739086 -1.7260866295903328

O -0.7833121522135728 2.7512786637647597 -1.304720254379945

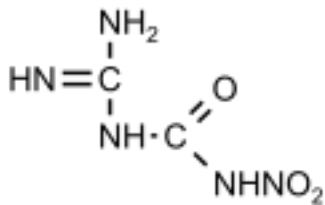
H 0.37593089577962024 0.7698057028426903 1.1133669092239136

H -1.4387809258082567 0.8993611367556078 0.6090491580661288

H 0.9435964704430913 0.11516565457689179 -1.1060167697271093

H -0.8706729014086134 0.254678549764376 -1.6092689912197

H -0.6621911131937572 -1.0244228697663598 1.7858753856553706



Chemical Name NITROGUANYLUREA

Molecular Formula (C2.0 H5.0 N5.0 O3.0)

Density(DICH)1.82(Ref.5)

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

Enthalpy of Formation(ENTH)-73.6(Ref.C)

Enthalpy of Formation(ENTH)-74.9(Ref.SE)

Melting Point(SCHM)245.0(Ref.ME1)

Melting Point(SCHM)415.0(Ref.1467)

Heat of Combustion(VBW)286.6(Ref.C)

Classification N.A

Oxygen Balance -38.07

Molecular Weight 147.093



