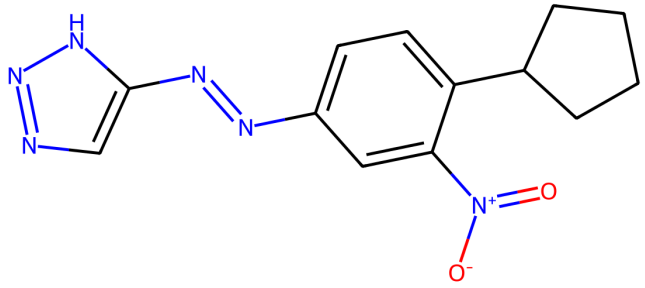
Thermal Hazard Assessment Memo

TestMol



Molecule Properties

SMILES: O=[N+]([O-])c1cc(/N=N/c2cnn[nH]2)ccc1C1CCCC1
Formula: 13C, 14H, 6N, 2O
MW: 286.30 g mol^{-1}
mp: 111.0 to 113.0 °C

Results

High Energy Groups: (3) N1C=CN=N1 |c:1,3|, CN=NC, C[N+](=O)[O-]

Explosive Groups: (3) CN=NC, N1C=CN=N1 |c:1,3|, C[N+](=O)[O-]

Rule of Six = 5 Oxygen Balance = -173.25

Q_{DSC} = 300.0 J g^{-1} T_{onset} = 330.0 °C T_{init} = 440.0 °C

Impact Sensitivity = -0.47 Explosive Propagation = -0.52 T_{D24} = 262.0 °C

O.R.E.O.S. assessment of risk by scale:

<5 g	5 to 100 g	100 to 500 g	>500 g
Medium Hazard	Medium Hazard	Medium Hazard	High Hazard

Interpretation

These results have been calculated using X^1 and they show Y^2.

[1]: *Org. Proc. Res. Dev.,* 2011, 2341-2356

[2]: *Org. Proc. Res. Dev.,* 2011, 2117-2119