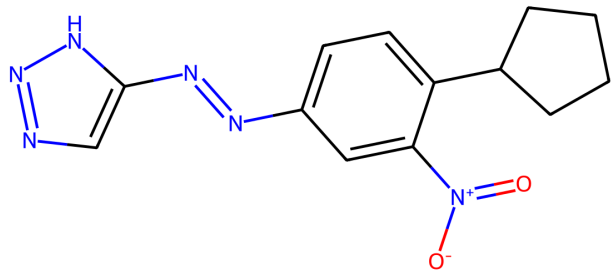
Thermal Hazard Assessment Memo

TestMol



Molecule Properties

SMILES: O=[N+]([O-])c1cc(/N=N/c2cnn[nH]2)ccc1C1CCCC1

Formula: 13C, 14H, 6N, 2O

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 = -173.24787369671137	
Q_{DSC} = 570.0 J g^{-1}	T_{onset} = 172.0	T_{init} = 222.0
Impact Sensitivity = -0.016068180950741473	Explosive Propagation = -0.15340226058995654	T_{D24} = 109.39999999999998 °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	High 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