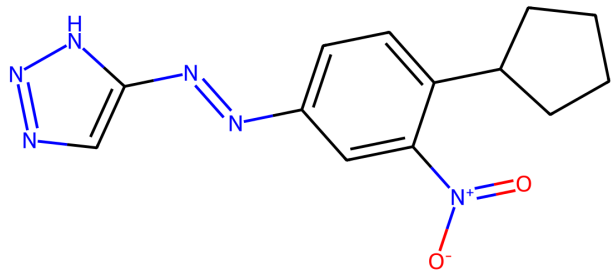
Thermal Hazard Assessment Memo

TestMol



Molecule Properties

SMILES: O=[N+]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

<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