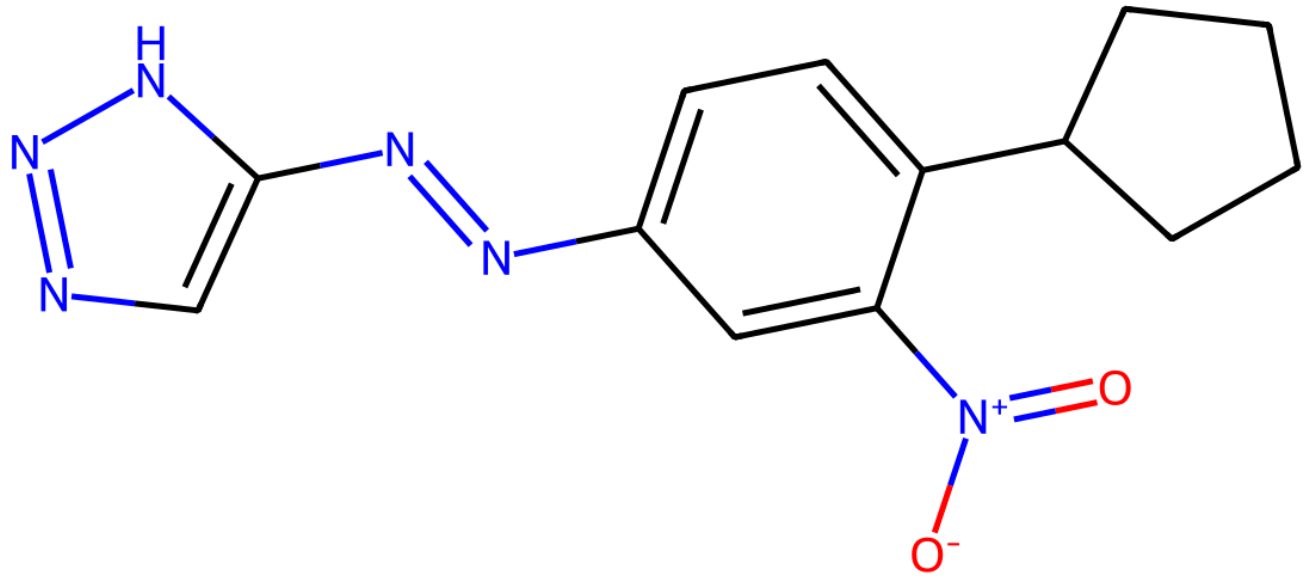
# Thermal Hazard Assessment Memo

## 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