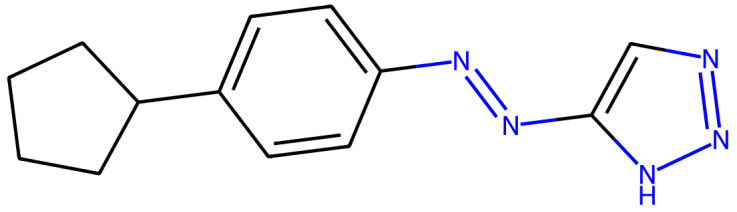
Thermal Hazard Assessment Memo

TestMol



Properties:

SMILES: c1cc(C2CCCC2)ccc1/N=N/c1cnn[nH]1

Name: TestMol

Formula: 13C, 15H, 5N

mp: 80 to 89 °C

Results:

High Energy Groups = 2 N1C=CN=N1 |c:1,3|, CN=NC

Explosive Groups = 2 CN=NC, N1C=CN=N1 |c:1,3|

Rule of Six = -1 Oxygen Balance = -222.13

Q_{DSC} = 990.00 J g⁻¹ T_{onset} = 91.00 °C T_{init} = 112.00 °C

Impact Sensitivity = 0.41 Explosive Propagation = 0.19 T_{D24} = 32.4 °C

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

Interpretation:

The Rule of Six[1] value imples (Not Explosive). The Oxygen Balance[1] suggests (Medium Risk)
The Pfizer method was used to calculate Impact Sensitivity and Explosive Propagation values, these suggest (Impact Sensitive) and (Propagates).
The T_{D24} result gives the maximum safe operation temperature.

[1] Org. Proc. Res. Dev., 2011, 2341-2356
[2] Org. Proc. Res. Dev., 2021, 2117-2119