Thermal Hazard Assessment Memo

MoreNitroTests

Properties:

SMILES: O=[N+]([O-])c1c(C2CCC2)cc2c(NO)cccc2c1[N+](=O)[O-]

Name: MoreNitroTests

Formula: 14C, 13H, 3N, 5O

mp: to °C

Results:

High Energy Groups = 3 CNO, C[N+](=O)[O-], C[N+](=O)[O-]

Explosive Groups = 3 CNO, C[N+](=O)[O-], C[N+](=O)[O-]

Rule of Six = 4 Oxygen Balance = -155.63

 $Q_{DSC} = 900.00 \text{ J g}^{-1}$ $T_{onset} = 140.00 \text{ °C}$ $T_{init} = 220.00 \text{ °C}$

Impact Sensitivity = 0.24 Explosive Propagation = 0.08 T_{D24} = 108.0 °C

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

Interpretation:

The Rule of Six¹ value imples (Explosive). The Oxygen Balance¹ suggests (Medium Risk). The Pfizer method² 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