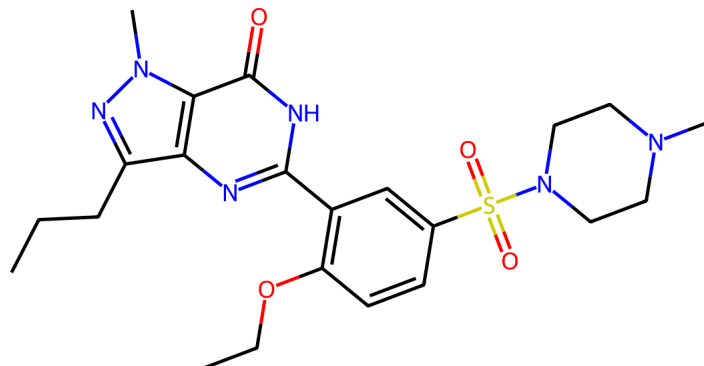# Thermal Hazard Assessment Memo

Properties:

SMILES: CCCC1=NN(C2=C1N=C(NC2=O)C3=C(C=CC(=C3)S(=O)(=O)N4CCN(CC4)C)OCC)C

Name:

Formula: 22C, 30H, 6N, 4O, S

mp: to None

Results:

High Energy Groups = 4 CNSC, C1=CNN=C1, C1=CN=CN=C1 |c:0,2,4|

Explosive Groups = 3 CNSC, C1=CN=CN=C1 |c:0,2,4|

Rule of Six = 2   Oxygen Balance = -185.42

Q_{DSC} T_{onset} T_{init}

Impact Sensitivity   Explosive Propagation T_{D24}

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

Interpretation:

The Rule of Six[1] value imples (Explosive). The Oxygen Balance[1] suggests (Medium Risk).
The Pfizer method was used to calculate Impact Sensitivity and Explosive Propagation values, these
suggest None and None.
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