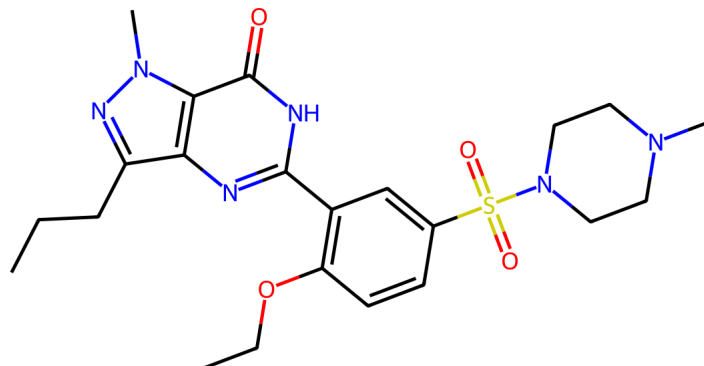


Thermal Hazard Assessment Memo

Sildenafil



Properties:

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

Name: Sildenafil

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

mp: 160 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

$Q_{DSC} = 360.00 \text{ J g}^{-1}$

$T_{onset} = 270.00 \text{ }^{\circ}\text{C}$

$T_{init} = 340.00 \text{ }^{\circ}\text{C}$

Impact Sensitivity = -0.34

Explosive Propagation = -0.42

$T_{D24} = 192.0 \text{ }^{\circ}\text{C}$

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

Interpretation:

The Rule of Six¹ value implies **(Explosive)**. The Oxygen Balance¹ suggests **(Medium Risk)**.

The Pfizer method was used to calculate Impact Sensitivity and Explosive Propagation values, these suggest **(Not Impact Sensitive)** and **(Should Not Propagate)**.

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