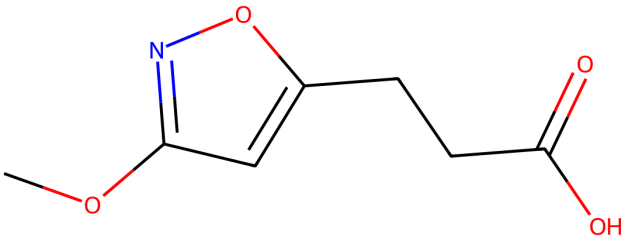
Thermal Hazard Assessment Memo



Molecule Properties

SMILES: COc1cc(CCC(=O)O)on1
Formula: 7C, 9H, N, 4O
MW: 171.15 g mol^{-1}

Results

High Energy Groups: (1) c1cnoc1

Explosive Groups: (1) c1cnoc1

Rule of Six = -1 Oxygen Balance = -135.55

Q_{DSC} = 421.0 J g^{-1} T_{onset} = 150.0 °C T_{init} = 110.0 °C

Impact Sensitivity = -0.11 Explosive Propagation = -0.26 T_{D24} = 31.00 °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	Medium Hazard	Medium 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