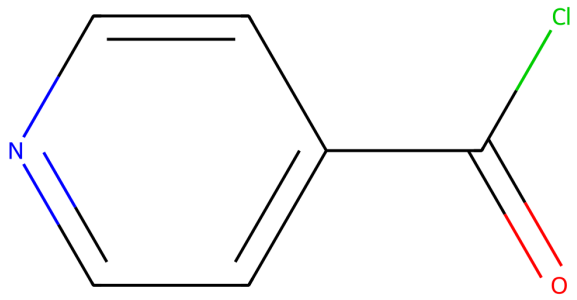
Thermal Hazard Assessment Memo

isonicotinoyl chloride



Molecule Properties

SMILES: O=C(Cl)c1ccncc1
Formula: 6C, 4H, Cl, N, O
MW: 141.56 g mol^{-1}
mp: 156.0 to 160.0 °C

Results

High Energy Groups: (0)

Explosive Groups: (0)

Rule of Six = -6 Oxygen Balance = -146.94

Q_{DSC} = 520.0 J g^{-1} T_{onset} = 225.0 °C T_{init} = 420.0 °C

Impact Sensitivity = -0.13 Explosive Propagation = -0.23 T_{D24} = 248.0 °C

O.R.E.O.S. assessment of risk by scale:

<5 g	5 to 100 g	100 to 500 g	>500 g
Low Hazard	Low Hazard	Low Hazard	Low Hazard

Interpretation

The 'Rule of Six'[1] is a simple metric that checks if there are at least 6 times as many carbon atoms as there are high energy functional groups in a molecule. The result above shows the result shows the diffrence beween 6 times the number of high energy groups vs the number of carbon atoms. As such a value of ≤ 0 implies that a compund should be safe to handel. Here the compound was found to be **(Not Explosive)** by this metric.

The 'Oxygen Balance'[1] is a method for assessing the explosive properties of molecules. The vaule is based on the carbon, hydrogen and oxygen content of a molecule and the MW. Using the oxygen balance the explosive risk can be assessed as 'High (OB -120 to 80)', 'Medium (OB 80 to 160, or -240 to -120)', or 'Low' (OB <-240 or >160). Here the risk is assessed as **(Medium Risk)**.

The likelyhood that a compound would exhibit impact sensitive or explosive propagation can be estimated from their 'Yoshida values'. These Yoshida values have been calculated using the Pfizer method from the Q_{DSC} and T_{onset} data.[2] If the Yoshida values are <0 the compound is not expected to exhibit that property. Here the molecule is expected to **not be impact sensitive** and to **not exhibit explosive propagation** based on these values.

T_{D24} is the temperature at which the time to the maximum rate of a runaway reaction is 24 h.[3] A reaction where the time to maximum rate is ≥ 24 h is highly unlikely to develop a thermal runaway. As such a reaction temperature of **248.0 °C or below** would be considered appropriate for this compound.

The O.R.E.O.S. assessment method assigns points based on the *O*xygen Balance, *R*ule of 6 value, presence of *E*xplosive functional groups, *O*nset temperature (T_{onset}), and reaction *S*cale.[1] As such two diffrent point scales are used depending on if a onset temperature is provided or not. Including T_{onset} data from DSC measurement is preferred. The table above provides the risk categories determined for this compound at 4 diffrent scales. Low Hazard results indicate reactions that can be performed using only the standard precautions. For use of compounds at scales that indicate Medium or High risk, discussion must be fist had with the process saftey team prior to any futher action. The O.R.E.O.S. value score for each scale was found to be:

<5 g	5 to 100 g	100 to 500 g	>500 g
10	11	13	17

[1]: *Org. Proc. Res. Dev.,* 2021, 25, 2, 212-224

[2]: *Org. Proc. Res. Dev.,* 2020, 24, 1, 67-84

[3]: *Angew. Chem. Int. Ed.,* 2020, 59, 15798-15802

Additional Data