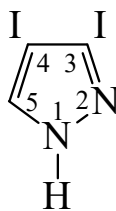




>>Entry Name: 3(5),4-Diiodopyrazole



CAS Registry Number: 6645-70-1

Molecular Formula: $C_3H_2I_2N_2$

Molecular Weight: 319.871

Accurate Mass: 319.830744

Percentage Composition: C 11.26%; H 0.63%; I 79.35%; N 8.76%

Physical Description: Needles (C_6H_6)

Melting Point: Mp 160-162°

>>Derivative: *N*-Ac

Molecular Formula: $C_5H_4I_2N_2O$

Molecular Weight: 361.908

Accurate Mass: 361.841309

Percentage Composition: C 16.59%; H 1.11%; I 70.13%; N 7.74%; O 4.42%

Physical Description: Cryst. (petrol)

Melting Point: Mp 83-85°

>>Derivative: *N*-Benzoyl

Molecular Formula: $C_{10}H_6I_2N_2O$

Molecular Weight: 423.979

Accurate Mass: 423.856959

Percentage Composition: C 28.33%; H 1.43%; I 59.86%; N 6.61%; O 3.77%

Physical Description: Cryst.

Melting Point: Mp 107-109°

>>Derivative: *N*-(4-Methylbenzenesulfonyl)

Physical Description: Cryst.

Melting Point: Mp 130-131°

>>Derivative: *N*-Benzyl

Molecular Formula: $C_{10}H_8I_2N_2$

Molecular Weight: 409.996

Accurate Mass: 409.877694

Percentage Composition: C 29.30%; H 1.97%; I 61.91%; N 6.83%

Physical Description: Cryst.

Melting Point: Mp 63-66°

References:

Giles, D. *et al.*, *J.C.S.(C)*, 1966, 1179, (*synth*)

Reimlinger, H. *et al.*, *Chem. Ber.*, 1970, **103**, 1942-1948, (*synth, ir, pmr*)

Holzer, W. *et al.*, *J. Het. Chem.*, 1995, **32**, 189, (*derivs*)