



>>Entry Name: 4-Iodo-3(5)-methylpyrazole

CAS Registry Number: 15802-75-2

Molecular Formula: C₄H₅IN₂

Molecular Weight: 208.001

Accurate Mass: 207.949746

Percentage Composition: C 23.10%; H 2.42%; I 61.01%; N 13.47%

Physical Description: Polyhedra (petrol); needles (EtOH)

Melting Point: Mp 110.5° (185-187°)

Refractive Index: n_D²⁰ 1.5670

>>Derivative: 1-Me

Synonym(s): 4-Iodo-1,3-dimethylpyrazole

CAS Registry Number: 6647-97-8

Molecular Formula: C₅H₇IN₂

Molecular Weight: 222.028

Accurate Mass: 221.965396

Percentage Composition: C 27.05%; H 3.18%; I 57.16%; N 12.62%

Physical Description: Yellow oil

Boiling Point: Bp₁₂ 107-108°

Refractive Index: n_D²⁰ 1.5670

>>Derivative: 2-Me

Synonym(s): 4-Iodo-1,5-dimethylpyrazole

CAS Registry Number: 6647-96-7

Molecular Formula: C₅H₇IN₂

Molecular Weight: 222.028

Accurate Mass: 221.965396

Percentage Composition: C 27.05%; H 3.18%; I 57.16%; N 12.62%

Physical Description: Needles (EtOH), cryst. (CCl₄)

Melting Point: Mp 113-113.5°

Other Data: Confused with 4-iodo-1,3-dimethylpyrazole. See note above

References:

Morgan, G.T. *et al.*, *J.C.S.*, 1923, **123**, 1308, (*synth*)

Hüttel, R. *et al.*, *Annalen*, 1955, **593**, 200, (*synth*)

Elguero, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1966, 3727, (*pmr*)

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

Sinyakov, A.N. *et al.*, *Bull. Acad. Sci. USSR, Div. Chem. Sci. (Engl. Transl.)*, 1977, 2142, (*derivs*)

Faure, R. *et al.*, *Can. J. Chem.*, 1988, **66**, 1141, (*cmr, tautom*)