



>>Entry Name: 5-Nitroindazole

CAS Registry Number: 5401-94-5

Molecular Formula: $C_7H_5N_3O_2$

Molecular Weight: 163.135

Accurate Mass: 163.038177

Percentage Composition: C 51.54%; H 3.09%; N 25.76%; O 19.61%

Physical Description: Leaflets or needles (EtOH)

Melting Point: Mp 208°

pKa Value: pK_{a1} 11.69 (25°)

Other Data: Spar. steam-volatile. Conc. alkali → red soln. → yellow on dilution

Aldrich: 21675-5

Fluka: 73409

>>Derivative: *N*-Ac

CAS Registry Number: 13436-55-0

Molecular Formula: $C_9H_7N_3O_3$

Molecular Weight: 205.173

Accurate Mass: 205.048742

Percentage Composition: C 52.69%; H 3.44%; N 20.48%; O 23.39%

Physical Description: 2 Forms: needles (EtOH) and needles (Me₂CO/Et₂O)

Melting Point: Mp 138-139°. Mp 158.9°

Other Data: Structs. not clear. Possibly 1-Ac and 2-Ac

>>Derivative: *N*-Benzoyl

CAS Registry Number: 23856-15-7

Molecular Formula: $C_{14}H_9N_3O_3$

Molecular Weight: 267.243

Accurate Mass: 267.064392

Percentage Composition: C 62.92%; H 3.39%; N 15.72%; O 17.96%

Physical Description: 2 Forms: leaflets (C₆H₆) and prisms (Me₂CO)

Melting Point: Mp 193-194°

>>Variant: 1*H*-form

Molecular Formula: $C_7H_5N_3O_2$

Molecular Weight: 163.135

Accurate Mass: 163.038177

Percentage Composition: C 51.54%; H 3.09%; N 25.76%; O 19.61%

>>Derivative: *N*-Me

Synonym(s): 1-Methyl-5-nitro-1*H*-indazole

CAS Registry Number: 5228-49-9

Molecular Formula: $C_8H_7N_3O_2$

Molecular Weight: 177.162

Accurate Mass: 177.053827

Percentage Composition: C 54.24%; H 3.98%; N 23.72%; O 18.06%

Physical Description: Pale-yellow needles (C₆H₆/petrol)

Melting Point: Mp 129°

>>Derivative: *N*-Me, methiodide

Physical Description: Golden yellow leaflets (H₂O)

Melting Point: Mp 203 dec.°

>>Derivative: *N*-Nitro

Synonym(s): 1,5-Dinitro-1*H*-indazole