>>**Entry Name: 6-Nitroindazole**

CAS Registry Number: 7597-18-4

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: Needles (toluene)
Melting Point: Mp 181°
pKa Value: pK_{a1} 11.67 (25°)

Aldrich: N1751-3

>>**Derivative:** *N*-Ac

CAS Registry Number: 13436-57-2
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: stable and labile leaflets (Et_2O)
Melting Point: Mp 140-141°. Mp 74-75°
Other Data: Structs. not clear, possibly 1-Ac and 2-Ac

>>**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*-Methoxycarbonyl

Molecular Formula: $C_9H_7N_3O_4$
Molecular Weight: 221.172
Accurate Mass: 221.043657
Percentage Composition: C 48.88%; H 3.19%; N 19.00%; O 28.94%
Physical Description: Yellow needles (MeOH)
Melting Point: Mp 169°

>>**Derivative:** *N*-Chlorocarbonyl

Molecular Formula: $C_8H_4ClN_3O_3$
Molecular Weight: 225.591
Accurate Mass: 224.994119
Percentage Composition: C 42.59%; H 1.79%; Cl 15.72%; N 18.63%; O 21.28%
Physical Description: Needles (Me_2CO)
Melting Point: Mp 140-141°
Solubility: Spar. sol. warm Et_2O

>>**Derivative:** *N*-Me
Synonym(s): 1-Methyl-6-nitro-1*H*-indazole

CAS Registry Number: 6850-23-3
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: Yellow needles (MeOH); cryst. (Et_2O/toluene)
Melting Point: Mp 108-109°. Mp 125°

>>**Derivative:** *N*-Me, methiodide