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>>Entry Name: 5-Nitro-1*H*-indole-3-carboxylic acid

CAS Registry Number: 6958-37-8

Molecular Formula: C<sub>9</sub>H<sub>6</sub>N<sub>2</sub>O<sub>4</sub>

Molecular Weight: 206.157

Accurate Mass: 206.032758

Percentage Composition: C 52.44%; H 2.93%; N 13.59%; O 31.04%

Physical Description: Solid

Melting Point: Mp 276-278 dec.° (256-258°)

>>Derivative: Amide

CAS Registry Number: 128200-32-8

Molecular Formula: C<sub>9</sub>H<sub>7</sub>N<sub>3</sub>O<sub>3</sub>

Molecular Weight: 205.173

Accurate Mass: 205.048742

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

Physical Description: Bright yellow solid

Melting Point: Mp 284-288°

>>Derivative: Nitrile

Synonym(s): 3-Cyano-5-nitroindole

CAS Registry Number: 7147-14-0

Molecular Formula: C<sub>9</sub>H<sub>5</sub>N<sub>3</sub>O<sub>2</sub>

Molecular Weight: 187.157

Accurate Mass: 187.038177

Percentage Composition: C 57.76%; H 2.69%; N 22.45%; O 17.10%

Physical Description: Cryst. (EtOAc/hexane)

Melting Point: Mp 186-190°

#### References:

Berti, G. *et al.*, *Gazz. Chim. Ital.*, 1961, **91**, 728, (*synth*)

Melzer, M.S. *et al.*, *J.O.C.*, 1962, **27**, 496, (*synth*)

Swain, C.J. *et al.*, *J. Med. Chem.*, 1992, **35**, 1019, (*synth, pmr*)