



>>Entry Name: 4-Amino-3-iodobenzoic acid

CAS Registry Number: 2122-63-6

Molecular Formula: $C_7H_6INO_2$

Molecular Weight: 263.034

Accurate Mass: 262.944327

Percentage Composition: C 31.96%; H 2.30%; I 48.25%; N 5.33%; O 12.17%

Physical Description: Yellow prisms (H_2O)

Melting Point: Mp 203-204°

pKa Value: pK_a 4.34

>>Derivative: N-Ac

Molecular Formula: $C_9H_8INO_3$

Molecular Weight: 305.072

Accurate Mass: 304.954892

Percentage Composition: C 35.43%; H 2.64%; I 41.60%; N 4.59%; O 15.73%

Physical Description: Needles (H_2O)

Melting Point: Mp 230°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2-iodoaniline

CAS Registry Number: 33348-34-4

Molecular Formula: $C_7H_5IN_2$

Molecular Weight: 244.034

Accurate Mass: 243.949746

Percentage Composition: C 34.45%; H 2.07%; I 52.00%; N 11.48%

Physical Description: Solid

Melting Point: Mp 94-97°

References:

Klemme, C.J. *et al.*, *J.O.C.*, 1940, **5**, 227

Goulette, G. *et al.*, *C. R. Hebd. Seances Acad. Sci. Ser. C*, 1975, **281**, 543

Kalfus, K. *et al.*, *Coll. Czech. Chem. Comm.*, 1975, **40**, 3009

Seydel, J.K. *et al.*, *J. Med. Chem.*, 1977, **20**, 439

Vaidyanathan, G. *et al.*, *J. Med. Chem.*, 1994, **37**, 3655, (nitrile synth, pmr, ms)