



>>Entry Name: 4-Azidobenzoic acid

CAS Registry Number: 6427-66-3

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%

Use/Importance: Intermed. for the synth. of photoaffinity labels

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 180-181°

Rare Chemicals Library: S6712-2

>>Derivative: Me ester

CAS Registry Number: 20442-96-0

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 leaflets (EtOH aq.)

Melting Point: Mp 39-40°

>>Derivative: Chloride

Molecular Formula: $C_7H_4ClN_3O$

Molecular Weight: 181.581

Accurate Mass: 181.004289

Percentage Composition: C 46.30%; H 2.22%; Cl 19.52%; N 23.14%; O 8.81%

Physical Description: Cryst. (hexane)

Melting Point: Mp 57-58°

References:

Rupe, H. *et al.*, *Ber.*, 1900, **33**, 3401, (*Me ester, synth*)

Rao, K.A.N. *et al.*, *J. Indian Chem. Soc.*, 1938, **15**, 194, (*synth*)

Pinney, K.G. *et al.*, *J.O.C.*, 1991, **56**, 3125, (*synth, chloride*)