



>>Entry Name: 1,4-Benzodioxan-6-carboxylic acid

Synonym(s): 2,3-Dihydro-1,4-benzodioxin-6-carboxylic acid. 3,4-Ethylenedioxybenzoic acid

CAS Registry Number: 4442-54-0

Molecular Formula: C₉H₈O₄

Molecular Weight: 180.16

Accurate Mass: 180.04226

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Physical Description: Needles (H₂O)

Melting Point: Mp 138-139°

>>Derivative: Me ester

CAS Registry Number: 20197-75-5

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Boiling Point: Bp_{1.5} 135-140° (lit. gives a pressure range)

>>Derivative: Chloride

CAS Registry Number: 6761-70-2

Molecular Formula: C₉H₇ClO₃

Molecular Weight: 198.605

Accurate Mass: 198.008372

Percentage Composition: C 54.43%; H 3.55%; Cl 17.85%; O 24.17%

Melting Point: Mp 102°

>>Derivative: Hydrazide

Molecular Formula: C₉H₁₀N₂O₃

Molecular Weight: 194.19

Accurate Mass: 194.069143

Percentage Composition: C 55.67%; H 5.19%; N 14.43%; O 24.72%

Physical Description: Needles (H₂O)

Melting Point: Mp 141°

References:

Heertjes, P.M. *et al.*, *J.C.S.*, 1957, 3445-3447, (*synth*)

Lipp, M. *et al.*, *Chem. Ber.*, 1958, **91**, 2247-2252, (*hydrazide*)

Byrne, M.M. *et al.*, *J.C.S.(B)*, 1968, 809-812, (*synth*)

Coudert, G. *et al.*, *Tet. Lett.*, 1978, 1059-1062, (*synth*)

Thurston, D.E. *et al.*, *J. Med. Chem.*, 1999, **42**, 1951-1964, (*synth, ir, pmr*)