



>>Entry Name: 4-Benzocyclobutenecarboxylic acid

Synonym(s): Bicyclo[4.2.0]octa-1,3,5-triene-3-carboxylic acid

CAS Registry Number: 875-94-5

Molecular Formula: C₉H₈O₂

Molecular Weight: 148.161

Accurate Mass: 148.05243

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Physical Description: Cryst. (petrol or H₂O)

Melting Point: Mp 139-140°

>>Derivative: Chloride

CAS Registry Number: 99718-03-3

Molecular Formula: C₉H₇ClO

Molecular Weight: 166.606

Accurate Mass: 166.018542

Percentage Composition: C 64.88%; H 4.23%; Cl 21.28%; O 9.60%

Physical Description: Pale-yellow oil

>>Derivative: Amide

Molecular Formula: C₉H₉NO

Molecular Weight: 147.176

Accurate Mass: 147.068414

Percentage Composition: C 73.45%; H 6.16%; N 9.52%; O 10.87%

Physical Description: Needles (H₂O)

Melting Point: Mp 142-143°

References:

Lloyd, J.B. *et al.*, *Tetrahedron*, 1964, **20**, 2185, (*synth*)

Horner, L. *et al.*, *Tet. Lett.*, 1965, 247, (*synth*)