



>>Entry Name: 1,4-Dihydroxy-2-naphthalenecarboxylic acid, 9Cl

Synonym(s): 1,4-Dihydroxy-2-naphthoic acid, 8Cl

CAS Registry Number: 31519-22-9

Structure by analogy with 1,3-Dihydroxy-2-naphthalenecarboxylic acid, [FNR60-M](#)

Molecular Formula: C₁₁H₈O₄

Molecular Weight: 204.182

Accurate Mass: 204.04226

Percentage Composition: C 64.71%; H 3.95%; O 31.34%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 200 (196°) dec.°

Aldrich: 28125-5

>>Derivative: Me ester

CAS Registry Number: 77060-74-3

Molecular Formula: C₁₂H₁₀O₄

Molecular Weight: 218.209

Accurate Mass: 218.05791

Percentage Composition: C 66.05%; H 4.62%; O 29.33%

Biological Source: Constit. of the fruit of *Rhoiptelea chiliantha*

Physical Description: Pale yellow granules

Melting Point: Mp 172-173°

>>Derivative: Et ester

CAS Registry Number: 66928-23-2

Molecular Formula: C₁₃H₁₂O₄

Molecular Weight: 232.235

Accurate Mass: 232.07356

Percentage Composition: C 67.23%; H 5.21%; O 27.56%

Physical Description: Oil

>>Derivative: 4-Me ether

Synonym(s): 1-Hydroxy-4-methoxy-2-naphthalenecarboxylic acid, 9Cl. 1-Hydroxy-4-methoxy-2-naphthoic acid

CAS Registry Number: 108170-53-2

Molecular Formula: C₁₂H₁₀O₄

Molecular Weight: 218.209

Accurate Mass: 218.05791

Percentage Composition: C 66.05%; H 4.62%; O 29.33%

Biological Source: Prod. by *Streptosporangium cinnabarinum*

Use/Importance: Herbicidal agent

Physical Description: Beige powder

UV: [neutral] λ_{max} 215 (); 261 (); 360 () (MeOH)

>>Derivative: Di-Me ether

Synonym(s): 1,4-Dimethoxy-2-naphthalenecarboxylic acid

CAS Registry Number: 78265-13-1

Molecular Formula: C₁₃H₁₂O₄

Molecular Weight: 232.235

Accurate Mass: 232.07356

Percentage Composition: C 67.23%; H 5.21%; O 27.56%

Melting Point: Mp 167-168°

References:

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Hauser, F.M. *et al.*, *J.O.C.*, 1978, **43**, 178
Brimble, M.A. *et al.*, *Aust. J. Chem.*, 1991, **44**, 197, (*synth, pmr*)
Pfefferle, C. *et al.*, *J. Antibiot.*, 1997, **50**, 1067-1068, (*isol, 4-Me ether*)
Brimble, M.A. *et al.*, *Tetrahedron*, 1998, **54**, 5363-5374, (*di-Me ether*)
Jiang, Z.-H. *et al.*, *Chem. Pharm. Bull.*, 2001, **49**, 737-740, (*Me ester, isol, pmr, cmr*)