



>>Entry Name: 6-Octene-2,4-diynedioic acid

Related CAS Registry Numbers(s): 3625-68-1

HOOCCH=CHC≡CC≡CCOOH

Molecular Formula: C<sub>8</sub>H<sub>4</sub>O<sub>4</sub>

Molecular Weight: 164.117

Accurate Mass: 164.01096

Percentage Composition: C 58.55%; H 2.46%; O 39.00%

>>Variant: (E)-form

Molecular Formula: C<sub>8</sub>H<sub>4</sub>O<sub>4</sub>

Molecular Weight: 164.117

Accurate Mass: 164.01096

Percentage Composition: C 58.55%; H 2.46%; O 39.00%

>>Derivative: 1-Monoamide

Synonym(s): Diatretin 1. Diatretyne I

Molecular Formula: C<sub>8</sub>H<sub>5</sub>NO<sub>3</sub>

Molecular Weight: 163.132

Accurate Mass: 163.026944

Percentage Composition: C 58.90%; H 3.09%; N 8.59%; O 29.42%

Biological Source: Prod. by *Clitocybe diatreta*, *Clitocybe cerussata*, *Clitocybe gallinacea* and *Clitocybe fragrans*

Physical Description: Cryst. (MeOH)

Melting Point: Mp 198° (explodes)

Solubility: BERDY SOL: Sol. MeOH, Et<sub>2</sub>O, bases; poorly sol. H<sub>2</sub>O, acids

UV: [neutral] λ<sub>max</sub> 223 (ε 37200); 260 (ε 11000); 275 (ε 16600); 291 (ε 23300); 310 (ε 18800) (EtOH) (Berdy)

Other Data: (E)-form assumed

Hazard & Toxicity: Explodes on melting ; BERDY HAZD : LD<sub>50</sub> (mus, ivn) 50 mg/kg

>>Derivative: 1-Mononitrile

Synonym(s): 7-Cyano-2-heptene-4,6-diynoic acid. **Diatretin 2.** Diatretyne II. Nudic acid B

CAS Registry Number: 463-15-0

Molecular Formula: C<sub>8</sub>H<sub>3</sub>NO<sub>2</sub>

Molecular Weight: 145.117

Accurate Mass: 145.016379

Percentage Composition: C 66.21%; H 2.08%; N 9.65%; O 22.05%

Biological Source: Prod. by *Clitocybe diatreta*, *Lepista dienii*, *Tricholoma nudium* and *Camarophyllus virgineus*

Physical Description: Cryst. (Et<sub>2</sub>O/petrol)

Melting Point: Mp 179-180 dec.°

Solubility: BERDY SOL: Sol. MeOH, bases, Et<sub>2</sub>O, Py; poorly sol. hexane, H<sub>2</sub>O, acids

UV: [neutral] λ<sub>max</sub> 231 (ε 46200); 239 (ε 58000); 268 (ε 7500); 285 (ε 14200); 304 (ε 20000); 322 (ε 14300) (MeOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD<sub>50</sub> (mus, ivn) 13 mg/kg

References:

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Anchel, M., *Arch. Biochem. Biophys.*, 1958, **78**, 100, (*isol*)

Ashworth, P.J. *et al.*, *J.C.S.*, 1958, 950, (*synth*)

Anchel, M. *et al.*, *Mycologia*, 1962, **54**, 249

Thaller, V. *et al.*, *J.C.S. Perkin 1*, 1972, 2032, (*isol, ms, nmr*)

Hearn, M.T.W. *et al.*, *J.C.S. Perkin 2*, 1976, 1027, (*cmr*)

Jones, E.R.H. *et al.*, *J. Chem. Res., Synop.*, 1981, 157, (*biosynth*)