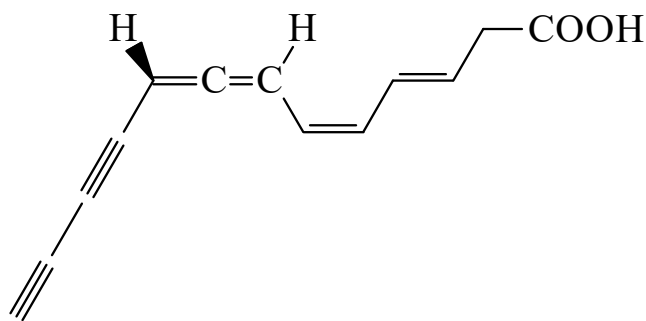




>>Entry Name: 3,5,7,8-Tridecatetraene-10,12-diynoic acid, 9Cl

Synonym(s): Mycomycin



CAS Registry Number: 544-51-4

Molecular Formula: C₁₃H₁₀O₂

Molecular Weight: 198.221

Accurate Mass: 198.06808

Percentage Composition: C 78.77%; H 5.08%; O 16.14%

UV: [neutral] λ_{max} 256 (sh) (ε 35000); 267 (ε 67000); 281 (ε 61000) (Et₂O) (Derep)

>>Variant: (3E,5Z)(R)-form

CAS Registry Number: 143789-07-5

Molecular Formula: C₁₃H₁₀O₂

Molecular Weight: 198.221

Accurate Mass: 198.06808

Percentage Composition: C 78.77%; H 5.08%; O 16.14%

Biological Source: Isol. from *Nocardia acidophilus*

Use/Importance: Antibiotic

Physical Description: Highly unstable solid

Melting Point: Mp 75° (explodes)

Optical Rotation: [α]_D²⁵ -130 (c, 0.4 in EtOH)

Solubility: BERDY SOL: Sol. MeOH, hexane; poorly sol. H₂O

UV: [neutral] λ_{max} 256 (ε 35000); 267 (ε 61000); 281 (ε 67000) (Et₂O) (Berdy)

Hazard & Toxicity: Explodes on melting ; BERDY HAZD : LD₅₀ (mus, ivn) 25 mg/kg

>>Derivative: Me ester

Physical Description: Cryst. (hexane)

Melting Point: Mp 44 dec.°

Optical Rotation: [α]_D²⁵ -120 (MeOH)

References:

Celmer, W.D. *et al.*, *J.A.C.S.*, 1952, **74**, 1870; 2245, (*isol, uv, ir, struct*)

Bohlmann, F. *et al.*, *Angew. Chem.*, 1964, **76**, 611, (*synth*)

Ahmed, M. *et al.*, *J. Chem. Res., Synop.*, 1977, 125, (*biosynth*)

Schlingmann, G. *et al.*, *J. Antibiot.*, 1995, **48**, 375, (*abs config*)