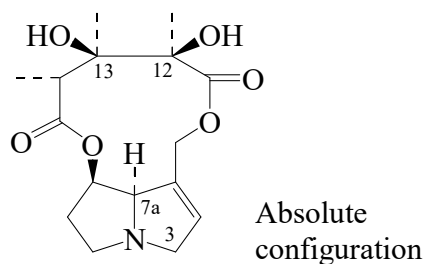




>>Entry Name: Monocrotaline

Synonym(s): 14,19-Dihydro-12,13-dihydroxy-20-norcrotalanan-11,15-dione, 9Cl



CAS Registry Number: 315-22-0

Molecular Formula: $C_{16}H_{23}NO_6$

Molecular Weight: 325.361

Accurate Mass: 325.152539

Percentage Composition: C 59.07%; H 7.12%; N 4.30%; O 29.50%

Biological Source: Alkaloid from *Crotalaria retusa*, *Crotalaria spectabilis*, *Crotalaria aegyptiaca*, *Crotalaria burhia* and *Lindelofia spectabilis* (Leguminosae, Boraginaceae)

Use/Importance: Hepatotoxin. Causative agent of much seneciosis, e.g. accidental poisoning by *S.* by weed residues in bread, and characterised by venooculosive disease.

Shows antineoplastic activity esp. vs. adenocarcinoma. Male insect sterilant. Used in China as an antineoplastic agent

Physical Description: Prisms (EtOH)

Melting Point: Mp 202-203° (197-198° dec.)

Optical Rotation: $[\alpha]_D^{26} -54.7$ (CHCl₃)

Calculated Log P Data: Log P -1.44 (uncertain value) (calc)

UV: [neutral] λ_{max} 217 (ϵ 20500) (MeOH) (Berdy)

Hazard & Toxicity: Exp. carcinogen. Possible human carcinogen. LD₅₀ (rat, orl) 66 mg/kg. Hepatotoxic

Aldrich: 27028-8

Fluka: 27975

Sigma: C2401

>>Derivative: Hydrochloride

Physical Description: Prisms (MeOH/CHCl₃)

Melting Point: Mp 184 dec.°

Optical Rotation: $[\alpha]_D^{28} -38.4$ (H₂O)

>>Derivative: Methiodide

Physical Description: Prisms (MeOH/CHCl₃)

Melting Point: Mp 205 dec.°

Optical Rotation: $[\alpha]_D^{28} +23.4$ (c, 3.1 in MeOH)

>>Derivative: N-Oxide

Synonym(s): Monocrotaline N-oxide

CAS Registry Number: 35337-98-5

Molecular Formula: $C_{16}H_{23}NO_7$

Molecular Weight: 341.36

Accurate Mass: 341.147454

Percentage Composition: C 56.30%; H 6.79%; N 4.10%; O 32.81%

Biological Source: Isol. from *Crotalaria sagittalis* (Leguminosae)

>>Derivative: O¹³-Ac

Synonym(s): Spectabiline†. Acetylmonocrotaline

CAS Registry Number: 520-55-8

Molecular Formula: $C_{18}H_{25}NO_7$

Molecular Weight: 367.398

Accurate Mass: 367.163104

Percentage Composition: C 58.85%; H 6.86%; N 3.81%; O 30.48%

Physical Description: Prisms (EtOH)

Melting Point: Mp 185.5-186°