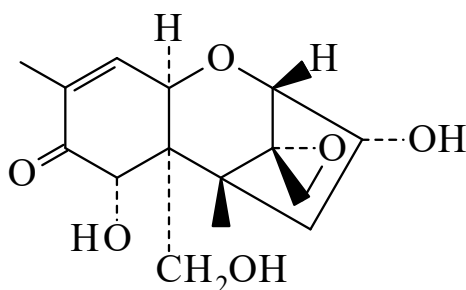




>>Entry Name: 3,7,15-Trihydroxy-8-scirpenone

ENTRY UNDER REVIEW

Synonym(s): 12,13-Epoxy-3,7,15-trihydroxy-9-trichothecen-8-one



Molecular Formula: C₁₅H₂₀O₆

Molecular Weight: 296.319

Accurate Mass: 296.12599

Percentage Composition: C 60.80%; H 6.80%; O 32.40%

>>Variant: (3 α ,7 α)-form

Synonym(s): Deoxynivalenol. Rd toxin. Vomitoxin

CAS Registry Number: 51481-10-8

Molecular Formula: C₁₅H₂₀O₆

Molecular Weight: 296.319

Accurate Mass: 296.12599

Percentage Composition: C 60.80%; H 6.80%; O 32.40%

Biological Source: Prod. by *Fusarium graminearum* and *Fusarium roseum*, responsible for headblight in cereals

Use/Importance: Mycotoxin. Emetric

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 151-153°

Optical Rotation: [α]_D²⁶ +6.35 (c, 0.07 in EtOH)

Hazard & Toxicity: Skin irritant. LD₅₀ (mus, orl) 46 mg/kg. Exp. reprod. and teratogenic effects. Associated with outbreaks of mycotoxicoses in farm animals

Sigma: D0156

Supelco: R47-4460

>>Derivative: Semicarbazone

Melting Point: Mp 199-201°

>>Derivative: 3-Ac

Synonym(s): Acetyldeoxynivalenol

CAS Registry Number: 50722-38-8

Molecular Formula: C₁₇H₂₂O₇

Molecular Weight: 338.357

Accurate Mass: 338.136555

Percentage Composition: C 60.35%; H 6.55%; O 33.10%

Biological Source: Toxin from infected barley

Physical Description: Cryst. (Et₂O/pentane)

Melting Point: Mp 185.5-186°

Optical Rotation: [α]_D +43 (c, 0.2 in MeOH)

UV: [neutral] $\lambda_{\max}$ 220 (ϵ 7100) (MeOH) [neutral] $\lambda_{\max}$ 220 (ϵ 7100) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 34 mg/kg

Sigma: A6166

>>Derivative: 3,7,15-Tri-Ac

Physical Description: Needles (EtOAc/petrol)

Melting Point: Mp 155-157°