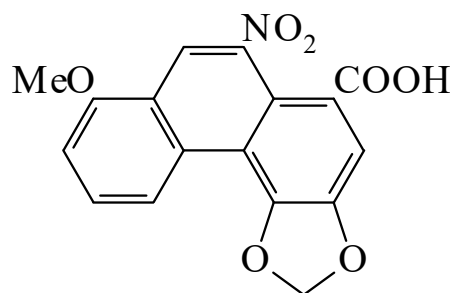




>>Entry Name: 8-Methoxy-3,4-methylenedioxy-10-nitro-1-phenanthrenecarboxylic acid

Synonym(s): 8-Methoxy-6-nitrophenanthro[3,4-*d*]-1,3-dioxole-5-carboxylic acid, 9Cl. **Aristolochic acid I**. Aristolochic acid A. Aristolochic acid. Isoaristolochic acid. **Aristolochin** $\ddagger$. Aristinic acid. Aristolochia yellow. Descressept. Tardolyt. TR 1736



CAS Registry Number: 313-67-7

Related CAS Registry Numbers(s): 10190-99-5

Molecular Formula: C₁₇H₁₁NO₇

Molecular Weight: 341.276

Accurate Mass: 341.053554

Percentage Composition: C 59.83%; H 3.25%; N 4.10%; O 32.82%

Biological Source: Alkaloid from a wide range of *Aristolochia* spp. Also found in the Chinese drug Fang-chi, *Asarum canadense* var. *reflexum*, *Bragantia wallichii*, and in the butterflies *Pachlioptera aristolochiae* and *Battus archidamas* (Aristolochiaceae)

Use/Importance: Phospholipase A₂ inhibitor. Antineoplastic, antiseptic, bactericidal agent. Antiinflammatory agent

Physical Description: Cryst. (DMF/EtOH, EtOH or MeOH/Et₂O)

Melting Point: Mp 281-286 dec.° (271-273°, 275-278°)

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

Calculated Log P Data: Log P 3.48 (calc)

UV: [base] λ_{max} 241 (ε); 305 (ε); 340 (ε); 450 (ε) (EtOH/NaOH) (Derep) [neutral] λ_{max} 221 (ε 29500); 255 (ε 32400); 283 (ε); 314 (ε 11200); 389 (ε 6030) (EtOH) (Derep) [neutral] λ_{max} 223 (ε 1174); 227 (ε 1148); 250 (ε 1445); 318 (ε 478); 390 (ε 251) (MeOH) (Berdy) [neutral] λ_{max} 221 (ε 29500); 250 (ε 32200); 317 (ε 11200); 390 (ε 6000) (EtOH) (Berdy)

Other Data: H₂SO₄ → green colour. λ_{max} 250 (ε 27000), 318 (12000) and 390 nm (6500)

Hazard & Toxicity: Nephrotoxic. Exp. carcinogen. LD₅₀ (rat, orl) 184 mg/kg. LD₅₀ (rat, ivn) 74 mg/kg

>>Derivative: Me ester

Synonym(s): Methyl aristolochate

CAS Registry Number: 1169-60-4

Molecular Formula: C₁₈H₁₃NO₇

Molecular Weight: 355.303

Accurate Mass: 355.069204

Percentage Composition: C 60.85%; H 3.69%; N 3.94%; O 31.52%

Biological Source: Alkaloid from roots of *Asarum indica* and *Asarum argentina* (Aristolochiaceae)

Physical Description: Yellow needles (CHCl₃/MeOH), cryst. (CHCl₃)

Melting Point: Mp 285-286° (281-282°)

References: