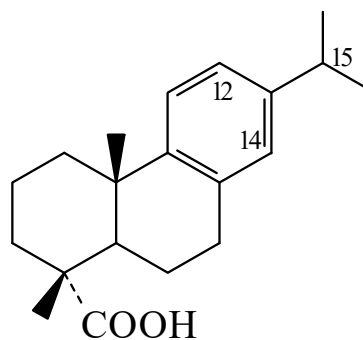




>>Entry Name: 8,11,13-Abietatrien-18-oic acid

Synonym(s): Dehydroabietic acid



CAS Registry Number: 1740-19-8

Molecular Formula: $C_{20}H_{28}O_2$

Molecular Weight: 300.44

Accurate Mass: 300.20893

Percentage Composition: C 79.96%; H 9.39%; O 10.65%

Biological Source: Constit. of *Pinus* and *Cedrus* spp. Also from *Abies sachalinensis* and *Cistus labdaniferus*

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 172-173°

Optical Rotation: $[\alpha]_D^{20} +62$ (EtOH)

UV: [neutral] λ_{max} 218 (); 243 (); 252 (); 270 (); 278 () (EtOH) (Berdy)

>>Derivative: Me ester

CAS Registry Number: 1235-74-1

Molecular Formula: $C_{21}H_{30}O_2$

Molecular Weight: 314.467

Accurate Mass: 314.22458

Percentage Composition: C 80.21%; H 9.62%; O 10.18%

Biological Source: Constit. of *Cistus labdaniferus* and *Pinus* spp.

Physical Description: Cryst. (EtOH)

Melting Point: Mp 62-63°

Boiling Point: $Bp_{0.2}$ 152-154°

Optical Rotation: $[\alpha]_D^{20} +60$ (EtOH)

>>Derivative: 12-Chloro

Synonym(s): 12-Chloro-8,11,13-abietatrien-18-oic acid. 12-Chlorodehydroabietic acid

CAS Registry Number: 65310-45-4

Molecular Formula: $C_{20}H_{27}ClO_2$

Molecular Weight: 334.885

Accurate Mass: 334.169957

Percentage Composition: C 71.73%; H 8.13%; Cl 10.59%; O 9.56%

Biological Source: Found in kraft papermill effluent

Use/Importance: Fish toxin

Physical Description: Cryst. (hexane)

Melting Point: Mp 178-180°

>>Derivative: 14-Chloro

Synonym(s): 14-Chloro-8,11,13-abietatrien-18-oic acid. 14-Chlorodehydroabietic acid

CAS Registry Number: 65281-76-7

Molecular Formula: $C_{20}H_{27}ClO_2$

Molecular Weight: 334.885

Accurate Mass: 334.169957

Percentage Composition: C 71.73%; H 8.13%; Cl 10.59%; O 9.56%

Biological Source: Found in kraft papermill effluent

Use/Importance: Fish toxicant

Physical Description: Cryst. (pentane)

Melting Point: Mp 159-160°