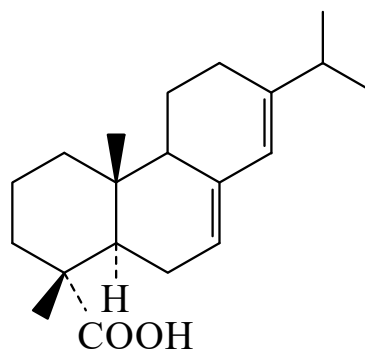




>>Entry Name: 7,13-Abietadien-18-oic acid

Synonym(s): Abietic acid



CAS Registry Number: 514-10-3

Related CAS Registry Numbers(s): 14351-66-7

Molecular Formula: C₂₀H₃₀O₂

Molecular Weight: 302.456

Accurate Mass: 302.22458

Percentage Composition: C 79.42%; H 10.00%; O 10.58%

Biological Source: Constit. of *Pinus* spp. Also from *Abies sibirica*, *Larix* spp., *Agathis* spp. and *Picea jezoensis*

Use/Importance: Used in metal soaps, additive in fermentations

Physical Description: Plates (EtOH)

Melting Point: Mp 171-173°

Optical Rotation: $[\alpha]_D^{15} -102$ (EtOH)

Solubility: BERDY SOL: Sol. MeOH, Et₂O; poorly sol. H₂O

UV: [neutral] $\lambda_{\max}$ 241 () (MeOH) (Berdy)

Other Data: The Abietic acid of commerce is often a resinous mixt. of acids obt. by acid isomerisation of pine resin. The major allergen in non-modified colophony

Hazard & Toxicity: LD₅₀ (mus, ivn) 180 mg/kg. Skin irritant and contact allergen

Aldrich: 16502-6

Fluka: 10

Sigma: A9424

>>Derivative: Me ester

CAS Registry Number: 127-25-3

Molecular Formula: C₂₁H₃₂O₂

Molecular Weight: 316.483

Accurate Mass: 316.24023

Percentage Composition: C 79.70%; H 10.19%; O 10.11%

Physical Description: Oil

Boiling Point: Bp₁ 170-180°

Optical Rotation: $[\alpha]_D -83.5$ (neat)

Density: d 1.05

Refractive Index: n_D^{20} 1.5286

Rare Chemicals Library: S64878-7

>>Derivative: Anhydride

Molecular Formula: C₄₀H₅₈O₃

Molecular Weight: 586.896

Accurate Mass: 586.438595

Percentage Composition: C 81.86%; H 9.96%; O 8.18%

Source/Synthesis: Formed in high-temperature rectification of pine resin. Minor constit. of coml. colophony

Melting Point: Mp 153-155°

>>Derivative: 7 α ,8 α :13 β ,14 β -Diepoxide

Synonym(s): 7,8:13,14-Diepoxo-18-abietanoic acid

CAS Registry Number: 338797-36-7

Molecular Formula: C₂₀H₃₀O₄

Molecular Weight: 334.455

Accurate Mass: 334.21441

Percentage Composition: C 71.82%; H 9.04%; O 19.13%

Biological Source: Constit. of *Larix kaempferi*

Physical Description: Needles (EtOAc/hexane)

Optical Rotation: $[\alpha]$