



Formula: C₂₀H₃₀O₂

MW: 302.46

CAS: 514-10-3

MDL: MFCD04220893

TNP: TNP00088



LogP: 0.36

LogS: -3.32

Acceptors: 2

Donors: 1

Rotation Bonds: 3

Chiral Centers: 4

N+O: 2

LIPINSKY: 4

IUPAC: (4bS,1R,10aR,4aR)-1,4a-dimethyl-7-(methylethyl)-1,2,3,4,5,6,10,10a,4a,4b-decahydrophenanthrenecarboxylic acid

Smiles: C1=2C([C]3(C(C(C(=O)O)(C)CCC3)CC2)C)CCC(C(C)C)=C1

Specification: Biochemistry; Terpenes (Others); Terpenes; Asymmetric Synthesis; Chiral Building Blocks; Complex Molecules ABIETIC ACID Chemical Properties:

mp 139-142 C(lit.) storage temp. 2-8C Sensitive Air Sensitive Merck 14,7 BRN 2221451 Stability:Stable. Combustible. Incompatible with strong oxidizing agents. CAS DataBase

Reference 514-10-3 (CAS DataBase Reference) Safety Information Hazard Codes Xi, N Risk Statements 36/37/38-50-50/53 Safety Statements 26-36 RIDADR UN 3077 9/PG 3 WGK Germany 3 RTECS TP8580000 F 10-23 ABIETIC ACID Usage And Synthesis Chemical Properties:

yellow resinous powder, crystals or chunks
General Description Yellowish resinous powder.
Reactivity Profile ABIETIC ACID reacts exothermically with bases, both organic (for example, the amines) and inorganic. Can react with active metals to form gaseous hydrogen and a metal salt. Such reactions are slow if the solid acid remains dry. Can react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slow for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H₂S and SO₃), dithionites (SO₂), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions.
Health Hazard ACUTE/CHRONIC HAZARDS: Slight fire hazard, slight explosive hazard as dust. Low toxicity. Fire Hazard Combustible. ABIETIC ACID Raw materials Turpentine oil

Merck 13 Reference: Monograph Number: 0000005

Title: Abietic Acid

CAS Registry Number: 514-10-3

CAS Name:

[1R-(1a,4ab,4ba,10aa)]-1,2,3,4,4a,4b,5,6,10,10a-Decahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenanthrenecarboxylic acid

Additional Names: 13-isopropylpodocarpa-7,13-dien-15-oic acid; sylvic acid

Molecular Formula: C₂₀H₃₀O₂

Molecular Weight: 302.45.

Percent Composition: C 79.42%, H 10.00%, O 10.58%

Literature References: A widely available organic acid, prepared by isomerization of rosin: Harris, Sanderson, *Org. Synth. coll. vol. IV*, 1 (1963); Fieser, Fieser, *The Chemistry of Natural Products Related to Phenanthrene* (New York, 3rd ed., 1949). Synthesis from dehydroabietic acid: A. W. Burgstahler, L. W. Worden, *J. Am. Chem. Soc.* 83, 2587 (1961); E. Wenkert et al., *ibid.* 86, 2038 (1964). Chromatographic study: A. G. Douglas, T. G. Powell, *J. Chromatogr.* 43,

241 (1969). Metabolism in rabbits: Y. Asakawa et al., *Xenobiotica* 16, 753 (1986).

Properties: Monoclinic plates from alcohol + water, mp 172-175. $[\alpha]_D^{24} -106$ (c = 1 in abs alc).
uv max: 235, 241.5, 250 nm (e 19500, 22000, 14300). Insol in water. Sol in alc, benzene, chloroform, ether, acetone, carbon disulfide, dil NaOH soln. Commercial abietic acid made by heating rosin alone or with acids may be glassy or partly crystalline, usually of yellow color and melting as low as 85.

Melting point: mp 172-175

Optical Rotation: $[\alpha]_D^{24} -106$ (c = 1 in abs alc)

Absorption maximum: uv max: 235, 241.5, 250 nm (e 19500, 22000, 14300)

Derivative Type: Methyl ester see Methyl Abietate

Use: Manufacture of esters (ester gums), e.g., methyl, vinyl and glyceryl esters for use in lacquers and varnishes. Manufacture of