



Formula: C₁₅H₂₀O₄

MW: 264.32

CAS: 21293-29-8

MDL: MFCD00075619

TNP: TNP00126



LogP: -1.89

LogS: -1.6

Acceptors: 4

Donors: 2

Rotation Bonds: 5

Chiral Centers: 1

N+O: 4

LIPINSKY: 4

IUPAC: (2Z,4E)-5-(1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-enyl)-3-methylpenta-2,4-dienoic acid

Smiles: C1(C(C(=CC(C1)=O)C)(O)C=CC(=CC(O)=O)C)(C)C

Merck 13 Reference: Monograph Number: 0000009

Title: Abscisic Acid

CAS Registry Number: 21293-29-8

CAS Name:
(2Z,4E)-5-[(1S)-Hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl]-3-methyl-2,4-pentadienoic acid

Additional Names: abscisin II; dormin; ABA

Molecular Formula: C₁₅H₂₀O₄

Molecular Weight: 264.32.

Percent Composition: C 68.16%, H 7.63%, O 24.21%

Literature References: Abscission-accelerating plant hormone; naturally occurring as the (+)-cis,trans-form. Regulates seed maturation and germination and mediates the plant response to environmental stress. Isolated from young cotton fruit: K. Ohkuma et al., *Science* 142, 1592 (1963); from sycamore leaves: J. W. Cornforth et al., *Nature* 205, 1269 (1965). Identification in sycamore, birch, rose, cabbage, potato, lemon, avocado: *idem*, *ibid.* 210, 627 (1966). Structure and synthesis of (