



Formula: C₁₈H₁₆O₈

MW: 360.32

CAS: 20283-92-5

TNP NUMBER: TNP00364

MDL NUMBER: MFCD02114256

IUPAC: 2-[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyloxy]-3-(3,4-dihydroxyphenyl)propanoic acid

Smiles: c1(ccc(cc1O)CC(OC(/C=Cc1ccc(c(c1)O)O)=O)C(=O)O)O

ACCEPTORS: 8

DONORS: 5

ROTATION BONDS: 12

N+O: 8

Chiral Centers: 1

LogP: 2.1

LogS: -3.66

LIPINSKI: 4

Synonyms: 3-(3,4-DIHYDROXYPHENYL)ACRYLIC
ACID-1-CARBOXY-2-(3,4-DIHYDROXYPHENYL)ETHYL
ESTER;ROSMARINATE;(R)-2-(3,4-DIHYDROXYCINNAMOYLOXY)-3-(3,4-DIHYDROXYPHEN
YL)LACTIC
ACID;(R)-A-[3-(3,4-DIHYDROXYPHENYL)-1-OXO-2E-PROPENYL]OXY-3,4-DIHYDROXYBEN
ZENEPROPANOIC
ACID;[R-(+)]-ALPHA-[[3-(3,4-DIHYDROXYPHENYL)-1-OXO-2-PROPENYL]OXY]-3,4-DIHYDR
OXYBENZENEPROPANOIC
ACID;(R)-ALPHA-[[3-(3,4-DIHYDROXYPHENYL)-1-OXO-2E-PROPENYL]OXY]-3,4-DIHYDRO
XY-BENZENEPROPANOIC
ACID;(2R)-3-(3,4-dihydroxyphenyl)-2-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy-propanoic
acid;3-(3,4-Dihydroxyphenyl)-2-[3-(3,4-dihydroxyphenyl)prop-2-enoyloxy]propanoic acid

CAS:537-15-5

MF:C18H16O8

MW:360.31

EINECS:

Product Categories: ROSMARINIC ACID

Chemical Properties: mp 171-175 C(lit.) Xi Risk Statements 36/38 Safety Statements
26-37/39 WGK Germany 3 RTECS GD8990000 F 10-23 ROSMARINIC ACID

Usage And Synthesis: ROSMARINIC ACID

