



Formula: C₁₈H₂₂O₄

MW: 302.37

CAS: 500-38-9

TNP NUMBER: TNP00263

MDL NUMBER: MFCD00002206

IUPAC: 4-[4-(3,4-dihydroxyphenyl)-2,3-dimethylbutyl]benzene-1,2-diol

Smiles: C(C(C(Cc1cc(O)c(cc1)O)C)C)c1cc(O)c(cc1)O

Occurs in as the meso-form in in the resinous exudate f the creosote bush, *Larrea divaricata*, Zygophyllaceae.

THERAPEUTIC CATEGORY: Antineoplastic

ACCEPTORS: 4

DONORS: 4

ROTATION BONDS: 9

N+O: 4

Chiral Centers: 2

LogP: 5.14

LogS: -4.63

LIPINSKI: 4

Synonyms: 1,2-Benzenediol,

4,4'-(2,3-dimethyl-1,4-butanediyl)bis-; 1,4-bis(3,4-dihydroxyphenyl)-2,3-dimethyl-butan; 2,3-Bis(3,4-dihydroxyphenylmethyl)butane; 4,4'-(2,3-Dimethyl-1,4-Butanediyl)bis(pyrocatechol); 4,4