



Formula: C<sub>25</sub>H<sub>28</sub>O<sub>3</sub>

MW: 376.5

CAS: 50-50-0

TNP NUMBER: TNP00604

MDL NUMBER: MFCD03548267

IUPAC: (1S,11S,14S,15S,10R)-14-hydroxy-15-methyltetracyclo[8.7.0.0.0]heptadeca-2,4,6-trien-5-yl benzoate

Smiles:

c12[C@H]3(CC[C]4([C@H]([C@@H]3(Cc1cc(OC(=O)c1ccccc1)cc2)))(CC[C@@H]4O))C

THERAPEUTIC CATEGORY: Estrogen

ACCEPTORS: 3

DONORS: 1

ROTATION BONDS: 2

N+O: 3

Chiral Centers: 5

LogP: 8.13

LogS: -6.21

LIPINSKI: 3

Synonyms: (17beta)-Estra-1,3,5(10)-triene-3,17-diol  
3-benzoate;1,3,5(10)-Estratriene-3,17-diol-3-benzoate;1,3,5(10)-Oestratriene-3,17-beta-diol  
3-benzoate;1,3,5(10)-oestratriene-3,17-beta-diol3-benzoate;17beta-Estradiol  
monobenzoate;17-beta-estradiolmonobenzoate;17-beta-Oestradiol  
3-benzoate;17-beta-oestradiol3-benzoate

CAS:50-50-0

MF:C25H28O3

MW:376.49

EINECS:200-043-7

Product Categories:Hormone;Biochemistry;Hydroxysteroids;Steroids Estradiol benzoate

Chemical Properties: mp 191-198 C(lit.) Merck 3703

CAS DataBase Reference: 50-50-0(

CAS DataBase Reference: ) NIST Chemistry ReferenceEstradiol benzoate(50-50-0) T Risk  
Statements 60-61-40 Safety Statements 53-22-36/37/39-45 WGK Germany 3 RTECS  
KG4050000 F 8 Hazardous Substances Data50-50-0(Hazardous Substances Data)  
1,3,5(10)-Estratriene-3,17b-diol 3-benzoate Estradiol benzoate

Usage And Synthesis: Estradiol benzoate

