



Formula: C₁₈H₂₀O₂

MW: 268.36

CAS: 474-86-2

TNP NUMBER: TNP00647

IUPAC: (11aS,6bS,8aS)-4-hydroxy-8a-methyl-2,7,8,10,11,11a,6b,8a-octahydrocyclopenta[1,2-a]phenanthren-9-one

Smiles: C1=2[C@H]3([C@](C(=O)CC3)(C)CC[C@@H]1(c1ccc(cc1CC2)O))

Steroidal Hormone isolated from urine of pregnant mares

THERAPEUTIC CATEGORY: Estrogen

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 1

N+O: 2

Chiral Centers: 3

LogP: 4.8

LogS: -4.6

LIPINSKI: 4

Synonyms:

1,3,5[10],7-ESTRATETRAEN-3-OL-17-ONE;3-HYDROXY-1,3,5[10],7-ESTRATETRAEN-17-ONE;7-DEHYDROESTRONE;EQUILIN;EQUILINE;1,3,5,7-estratetraen-3-ol-17-one;3-Hydroxyestra-1,3,5(10),7-tetraen-17-one;5(10),7-tetraen-17-one,3-hydroxy-estra-3

CAS:474-86-2

MF:C18H20O2

MW:268.35

EINECS:207-488-6

Product Categories: EQUILIN

Chemical Properties: mp 238-240 C(lit.) Merck 13,3672 Xn Risk Statements 40-62-63 Safety Statements 36/37 WGK Germany 3 RTECS KG6650000 EQUILIN

Usage And Synthesis: EQUILIN

