



Formula: C₁₈H₂₀O₂

MW: 268.36

CAS: 6898-97-1

MDL NUMBER: MFCD00870590

IUPAC: 4-[(1Z)-1-ethyl-2-(4-hydroxyphenyl)but-1-enyl]phenol

Smiles: C(=C(/c1ccc(cc1)O)CC)/(c1ccc(cc1)O)CC

Banned by FDA in 1979 as a growth promotant in livestock. Antibacterial properties see in: G.H. Faulkner, Biochem, 1944, 38, p.371.

THERAPEUTIC CATEGORY: ESTROGEN; Antibacterial

REFERENCE: SanMarti'n S, et al. Effects of diethylstilbestrol on mouse hippocampal evoked potentials in vitro. Cell Mol Neurobiol. 1999 Dec;19(6):691-703 Sunny F, Oommen OV. Rapid action of testosterone and diethylstilbestrol on enzymes of osmoregulation in a freshwater fish *Oreochromis mossambicus*. Endocr Res. 2002 Feb-May;28(1-2):69-81 Turner RT, et al. Mechanism of action of estrogen on cancellous bone balance in tibiae of ovariectomized growing rats: inhibition of indices of formation and resorption. J Bone Miner Res. 1993 Mar;8(3):359-66

SOURCE: Synthetic estrogen

ACCEPTORS: 2

DONORS: 2

ROTATION BONDS: 4

N+O: 2

Chiral Centers: 0

LogP: 5.95

LogS: -4.82

LIPINSKI: 4

Synonyms: DIETHYLSTILBESTROL 97% MIXTURE OF CIS&diethylstilbestrol, mixture of cis and trans;Diethylstilbestrol,mixture of cis and trans;DIETHYLSTILBESTROL, 99%, MIXTURE OF CIS AND TRANS;4,4'-Hex-3-ene-3,4-diylidiphenol;DES;Diethylstilbestrol;3,4-Bis(4-hydroxyphenyl)-3-hexene

CAS:6898-97-1

MF:C18H20O2

MW:268.35

EINECS:200-278-5

Product Categories:Stilbenes Diethylstilbestrol

Chemical Properties: mp 170-172 C(lit.) Merck 3129 T,N Risk Statements 45-61-36/37/38-51/53 Safety Statements 53-36/37/39-45-60-61 RIDADR UN 3077 9/PG 3 WGK Germany 3 RTECS WJ560000 Diethylstilbestrol

Usage And Synthesis: Diethylstilbestrol

