



Formula: C₁₈H₂₂O₂

MW: 270.37

CAS: 84-16-2

MDL NUMBER: MFCD00068996

IUPAC: 4-[(2S,1R)-1-ethyl-2-(4-hydroxyphenyl)butyl]phenol

Smiles: c1([C@@H]([C@@H](c2ccc(cc2)O)CC)CC)ccc(cc1)O

G.H. Faulkner, Biochem, 1944, 38, p.371.

THERAPEUTIC CATEGORY: Estrogen, Antineoplastic, Antibacterial

VET THERAP CATEGORY: ESTROGEN

ACCEPTORS: 2

DONORS: 2

ROTATION BONDS: 3

N+O: 2

Chiral Centers: 2

LogP: 6.12

LogS: -4.91

LIPINSKI: 3

Monograph Number: 0004720

Title: Hexestrol

CAS Registry Number: 84-16-2

CAS Name: 4,4