



Accurate Mass: 382.21441
Percentage Composition: C 75.36%; H 7.91%; O 16.73%
Use/Importance: Estrogen
Physical Description: Cryst. (petrol)
Melting Point: Mp 127-128°
Calculated Log P Data: Log P 6.2 (calc)
Sigma: H8387

>>**Derivative:** Dioctanoyl
Synonym(s): Hexestrol dicaprylate. Taston

CAS Registry Number: 20305-51-5

Use/Importance: Estrogen
Calculated Log P Data: Log P 11.49 (uncertain value) (calc)

>>**Derivative:** Bis[4-[bis(2-chloroethyl)amino]phenylacetate]
Synonym(s): Phenestrol

CAS Registry Number: 19659-38-2

Molecular Formula: C₄₂H₄₈Cl₄N₂O₄
Molecular Weight: 786.663
Accurate Mass: 784.236816
Percentage Composition: C 64.13%; H 6.15%; Cl 18.03%; N 3.56%; O 8.14%
Use/Importance: Antineoplastic agent
Physical Description: Cryst. (Me₂CO)
Melting Point: Mp 144-146°
Calculated Log P Data: Log P 11.28 (uncertain value) (calc)

>>**Derivative:** Bis(2-diethylaminoethyl)ether
Synonym(s): Coralgil. Diethyphen. Many other names

CAS Registry Number: 2691-45-4

Use/Importance: Coronary vasodilator
Calculated Log P Data: Log P 8.24 (uncertain value) (calc)
Hazard & Toxicity: Causes phospholipidosis of liver and lung cells and foam cell syndrome. Use discontinued since 1970

>>**Derivative:** Bis(2-diethylaminoethyl)ether, hydrochloride (1:2)

CAS Registry Number: 69-14-7
Physical Description: Needles (EtOH/EtOAc)
Melting Point: Mp 226-227°

>>**Variant:** (3*RS*,4*SR*)-form
Synonym(s): *meso*-form

CAS Registry Number: 84-16-2
Molecular Formula: C₁₈H₂₂O₂
Molecular Weight: 270.371
Accurate Mass: 270.16198
Percentage Composition: C 79.96%; H 8.20%; O 11.84%
Use/Importance: Highly active nonsteroidal estrogen with potency similar to that of Estrone [HLF43-J](#) and Estradiol (see Estra-1,3,5(10)-triene-3,17-diol [BBB24-E](#))
Physical Description: Needles (C₆H₆)
Melting Point: Mp 185-186°
Hazard & Toxicity: LD₅₀ (mus, orl) 1000 mg/kg. Exp. reprod. and teratogenic effects. Exp. hepatotoxic and haematological effects. Cytotoxic (inhibits microtubule assembly)

Aldrich: 21968-1
Rare Chemicals Library: S56055-3
Sigma: H7753