



Molecular Formula: C₁₉H₂₆O₃
Molecular Weight: 302.413
Accurate Mass: 302.188195
Percentage Composition: C 75.46%; H 8.67%; O 15.87%
Physical Description: Cryst. (C₆H₆)
Melting Point: Mp 192-192.5°

>>Derivative: 3,16-Di-Me ether

CAS Registry Number: 24185-75-9
Physical Description: Cryst. (MeOH aq.)
Melting Point: Mp 139-140.5°

>>Derivative: 3,17-Di-Me ether

Synonym(s): 3,17β-Dimethoxyestra-1,3,5(10)-trien-16α-ol

CAS Registry Number: 17292-36-3

Molecular Formula: C₂₀H₂₈O₃
Molecular Weight: 316.439
Accurate Mass: 316.203845
Percentage Composition: C 75.91%; H 8.92%; O 15.17%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 168-169.5°
Optical Rotation: [α]_D²⁴+41 (c, 0.6 in CHCl₃)

>>Derivative: Tri-Me ether

CAS Registry Number: 21099-66-1

Physical Description: Cryst. (MeOH)
Melting Point: Mp 110°
Optical Rotation: [α]_D+57 (CHCl₃)

>>Derivative: 3-Cyclopentyl ether

Synonym(s): Quinestradol, BAN, INN. Quinestradiol. Colpovis. Colpovister. Pentovis

CAS Registry Number: 1169-79-5

Molecular Formula: C₂₃H₃₂O₃
Molecular Weight: 356.504
Accurate Mass: 356.235145
Percentage Composition: C 77.49%; H 9.05%; O 13.46%
Use/Importance: Estrogen
Physical Description: Cryst. (Et₂O/hexane)
Melting Point: Mp 161-162°
Optical Rotation: [α]_D+47 (dioxan)

>>Derivative: 3-O-β-D-Glucuronopyranoside

Synonym(s): Estriol 3-glucosiduronic acid

CAS Registry Number: 2479-91-6

Extra CAS Registry Numbers(s): 28808-07-3

Molecular Formula: C₂₄H₃₂O₉
Molecular Weight: 464.511
Accurate Mass: 464.204635
Percentage Composition: C 62.06%; H 6.94%; O 31.00%
Physical Description: Leaflets
Melting Point: Mp 213-220° (dec.)
Optical Rotation: [α]_D¹⁶-18.1 (c, 0.05 in EtOH)