



Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 116-117.5°

>>**Derivative:** Tri-Me ether

Synonym(s): 3,16 α ,17 α -Trimethoxyestra-1,3,5(10)-triene

CAS Registry Number: 20796-64-9

Molecular Formula: C₂₁H₃₀O₃

Molecular Weight: 330.466

Accurate Mass: 330.219495

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Physical Description: Cryst (MeOH aq.)

Melting Point: Mp 80-82°

>>**Variant:** (16 α ,17 β OH)-form

Synonym(s): Estriol. Oestriol, BAN. Folliculin. Holin V. Ovestin. Thelol. NSC 12169. Many other names

CAS Registry Number: 50-27-1

Molecular Formula: C₁₈H₂₄O₃

Molecular Weight: 288.386

Accurate Mass: 288.172545

Percentage Composition: C 74.97%; H 8.39%; O 16.64%

Use/Importance: Used in estrogen replacement therapy

Physical Description: Cryst.

Melting Point: Mp 214.6°

Calculated Log P Data: Log P 2.55 (uncertain value) (calc)

Hazard & Toxicity: Exp. neoplastic agent and teratogen

Aldrich: 28580-3

Fluka: 75292

Sigma: E1253

>>**Derivative:** 3-Ac

CAS Registry Number: 17779-98-5

Molecular Formula: C₂₀H₂₆O₄

Molecular Weight: 330.423

Accurate Mass: 330.18311

Percentage Composition: C 72.70%; H 7.93%; O 19.37%

Physical Description: Prisms (C₆H₆)

Melting Point: Mp 184-187°

Optical Rotation: [α]_D²¹+54.4 (c, 0.85 in CHCl₃)

>>**Derivative:** 16-Ac

CAS Registry Number: 853-24-7

Molecular Formula: C₂₀H₂₆O₄

Molecular Weight: 330.423

Accurate Mass: 330.18311

Percentage Composition: C 72.70%; H 7.93%; O 19.37%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 198-200°

Optical Rotation: [α]_D²⁰+38 (c, 0.6 in dioxan)

>>**Derivative:** 3,16-Di-Ac

Molecular Formula: C₂₂H₂₈O₅

Molecular Weight: 372.46

Accurate Mass: 372.193675

Percentage Composition: C 70.95%; H 7.58%; O 21.48%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 155-157°