



>>Entry Name: 17-Hydroxy-19-norpregn-4-ene-3,20-dione, 9CI

Molecular Formula: C₂₀H₂₈O₃
Molecular Weight: 316.439
Accurate Mass: 316.203845
Percentage Composition: C 75.91%; H 8.92%; O 15.17%

>>Variant: (17 α OH)-form

CAS Registry Number: 2137-18-0
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. (Me₂CO/hexane)
Melting Point: Mp 204-206°
Optical Rotation: [α]_D +41 (CHCl₃)

>>Derivative: Me ether

Synonym(s): 17 α -Methoxy-19-norpregn-4-ene-3,20-dione

CAS Registry Number: 40803-71-2

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. (Me₂CO/hexane)
Melting Point: Mp 151-152°
Optical Rotation: [α]_D²⁵ +106.8 (c, 0.5 in CHCl₃)

>>Derivative: Ac

CAS Registry Number: 31981-44-9
Molecular Formula: C₂₂H₃₀O₄
Molecular Weight: 358.477
Accurate Mass: 358.21441
Percentage Composition: C 73.71%; H 8.43%; O 17.85%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 227-229°
Optical Rotation: [α]_D²⁵ +22 (c, 0.518 in CHCl₃)

>>Derivative: 17-Sulfate

Melting Point: Mp 152-155° (as Na salt)
Optical Rotation: [α]_D²² +63.7 (MeOH) (as Na salt)

>>Variant: (17 β OH)-form

CAS Registry Number: 16895-64-0
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. (Me₂CO/hexane)
Melting Point: Mp 142.1°
Optical Rotation: [α]_D²⁵ +36 (c, 0.5 in CHCl₃)

>>Derivative: Ac

CAS Registry Number: 66964-58-7
Physical Description: Cryst. (Me₂CO/hexane)
Melting Point: Mp 174.3°
Optical Rotation: [α]_D²⁵ +29.2 (c, 0.5 in CHCl₃)