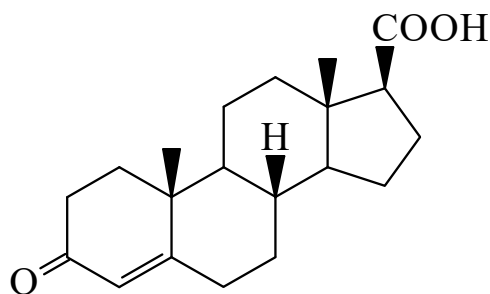




>>Entry Name: 3-Oxoandrost-4-ene-17-carboxylic acid, 9Cl

Synonym(s): 3-Oxoeti-4-enic acid



Related CAS Registry Numbers(s): 73835-78-6 73838-03-6

Molecular Formula: C₂₀H₂₈O₃

Molecular Weight: 316.439

Accurate Mass: 316.203845

Percentage Composition: C 75.91%; H 8.92%; O 15.17%

Other Data: (±)-17 α and (±)-17 β forms also known

>>Variant: 17 β -form

Synonym(s): Etienic acid

CAS Registry Number: 302-97-6

Molecular Formula: C₂₀H₂₈O₃

Molecular Weight: 316.439

Accurate Mass: 316.203845

Percentage Composition: C 75.91%; H 8.92%; O 15.17%

Source/Synthesis: Semisynth. steroid prod. from the corresponding 17 β -methylbutyric acid by incubating with *Proactinomyces erythropolis*

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 246-250°

Optical Rotation: [α]_D +163 (c, 1 in CHCl₃)

>>Derivative: Nitrile

CAS Registry Number: 63079-23-2

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 170-171°

Optical Rotation: [α]_D²⁰ -162 (CHCl₃)

>>Derivative: Amide

CAS Registry Number: 92472-22-5

Molecular Formula: C₂₀H₂₉NO₂

Molecular Weight: 315.455

Accurate Mass: 315.219829

Percentage Composition: C 76.15%; H 9.27%; N 4.44%; O 10.14%

Physical Description: Cryst. (hexane/toluene)

Melting Point: Mp 261-263°

>>Derivative: Me ester

CAS Registry Number: 2681-55-2

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. (Et₂O/pentane)

Melting Point: Mp 133-134°

>>Derivative: 20-O- β -D-Glucopyranosiduronic acid

Molecular Formula: C₂₆H₃₆O₉

Molecular Weight: 492.565

Accurate Mass: 492.235935

Percentage Composition: C 63.40%; H 7.37%; O 29.23%

Optical Rotation: [α]_D²⁶ +113 (MeOH) (as Me ester)