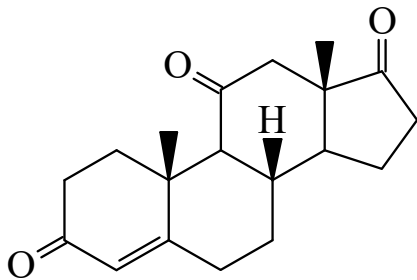




>>Entry Name: Androst-4-ene-3,11,17-trione, 9Cl
Synonym(s): Adrenosterone. Reichstein's substance G



CAS Registry Number: 382-45-6

Molecular Formula: C₁₉H₂₄O₃
Molecular Weight: 300.397
Accurate Mass: 300.172545
Percentage Composition: C 75.97%; H 8.05%; O 15.98%
Biological Source: Constit. of the adrenal cortex
Use/Importance: Aromatase (estrogen synthetase) inhibitor. Male sex hormone
Physical Description: Plates (EtOH) or needles
Melting Point: Mp 224-226° (220-224°)
Optical Rotation: [α]_D +350 (CHCl₃)
Calculated Log P Data: Log P 0.88 (uncertain value) (calc)

Aldrich: 28499-8
Rare Chemicals Library: S35733-2
Sigma: A6252

>>Derivative: 17-Oxime

Molecular Formula: C₁₉H₂₅NO₃
Molecular Weight: 315.411
Accurate Mass: 315.183444
Percentage Composition: C 72.35%; H 7.99%; N 4.44%; O 15.22%
Physical Description: Cryst. (Me₂CO)
Melting Point: Mp 250-252°
Optical Rotation: [α]_D³³ +158.7 (CHCl₃)

>>Derivative: 3,17-Dioxime

Molecular Formula: C₁₉H₂₆N₂O₃
Molecular Weight: 330.426
Accurate Mass: 330.194343
Percentage Composition: C 69.07%; H 7.93%; N 8.48%; O 14.53%
Physical Description: Cryst. (Me₂CO/Et₂O)
Melting Point: Mp 156-157°
Optical Rotation: [α]_D²⁴ +207 (CHCl₃)

>>Variant: (9 β ,10 α)-form

Molecular Formula: C₁₉H₂₄O₃
Molecular Weight: 300.397
Accurate Mass: 300.172545
Percentage Composition: C 75.97%; H 8.05%; O 15.98%
Physical Description: Cryst. (Me₂CO/diisopropyl ether)
Melting Point: Mp 184-185°
Optical Rotation: [α]_D²⁵ +64 (c, 0.1 in dioxan). [α]_D²⁵ +84.5 (CHCl₃)

>>Variant: 10 α -form

CAS Registry Number: 15407-71-3
Molecular Formula: C₁₉H₂₄O₃
Molecular Weight: 300.397
Accurate Mass: 300.172545
Percentage Composition: C 75.97%; H 8.05%; O 15.98%
Physical Description: Cryst. (Me₂CO/hexane)
Melting Point: Mp 177-178°
Optical Rotation: [α]