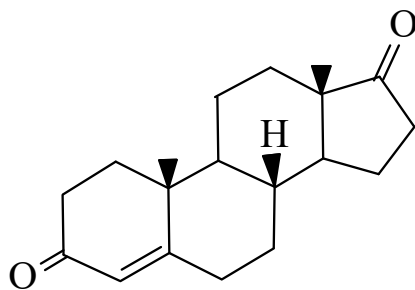




>> Name: **Androst-4-ene-3,17-dione**

Synonym(s): Androstenedione. Fecundin. Androtex



CAS Registry Number: 63-05-8

Related CAS Registry Numbers(s): 1927-34-0 2243-19-8 4419-89-0 4860-73-5 13864-55-6 34751-00-3 41143-27-5 58130-56-6 61074-03-1 61856-05-1 63893-25-4 67034-84-8 67034-85-9 67110-83-2 70585-32-9 71995-66-9 71995-67-0 71995-68-1 79037-28-8 79298-23-0 83118-38-1 88719-10-2 88980-25-0 88980-26-1 97143-49-2 97473-93-3 97473-94-4 97473-95-5 97473-96-6 103845-52-9

Molecular Formula:  $C_{19}H_{26}O_2$

Molecular Weight: 286.413

Accurate Mass: 286.19328

Percentage Composition: C 79.68%; H 9.15%; O 11.17%

Biological Source: Occurs in numerous tissues as hormonal metab. Urine constit. Obtainable by microbial fermentation routes

Use/Importance: Natural precursor in biosynth. of estrogens and testosterone. Conversion to estrogens by aromatase may be inhibited by aromatase inhibitors, and these are used in the treatment of estrogen-dependent disorders

Physical Description: Cryst. (hexane)

Melting Point: Mp 173-174°

Optical Rotation:  $[\alpha]_D^{18} +185$  (EtOH).  $[\alpha]_D +194$  (CHCl<sub>3</sub>)

Other Data: Deuterated and tritiated compds. have been synth. Also exists in 2 polymorphic forms, Mp 126-129° and Mp 135-138°

Hazard & Toxicity: Exp. teratogen, causes exp. neoplasms

Aldrich: 28513-7

Fluka: 10340

Rare Chemicals Library: S35798-7

Sigma: A9630

>>Variant: 9 $\beta$ -form

CAS Registry Number: 846-47-9

Molecular Formula:  $C_{19}H_{26}O_2$

Molecular Weight: 286.413

Accurate Mass: 286.19328

Percentage Composition: C 79.68%; H 9.15%; O 11.17%

Physical Description: Cryst. (Et<sub>2</sub>O)

Melting Point: Mp 124-125°

Optical Rotation:  $[\alpha]_D^{25} +172$  (CHCl<sub>3</sub>)

>>Variant: (9 $\beta$ ,10 $\alpha$ )-form

CAS Registry Number: 571-45-9

Molecular Formula:  $C_{19}H_{26}O_2$

Molecular Weight: 286.413

Accurate Mass: 286.19328

Percentage Composition: C 79.68%; H 9.15%; O 11.17%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 154-156°

>>Variant: (9 $\beta$ ,10 $\alpha$ ,13 $\alpha$ )-form

CAS Registry Number: 79732-29-9

Molecular Formula:  $C_{19}H_{26}O_2$

Molecular Weight: 286.413

Accurate Mass: 286.19328

Percentage Composition: C 79.68%; H 9.15%; O 11.17%

Physical Description: Cryst. (CH<sub>2</sub>Cl<sub>2</sub>/petrol)

Melting Point: Mp 90-91°

Optical Rotation:  $[\alpha]_D -176$  (c, 0.1 in dioxan)