



>>Entry Name: Androst-3-en-17-one

Molecular Formula: C₁₉H₂₈O

Molecular Weight: 272.43

Accurate Mass: 272.214015

Percentage Composition: C 83.77%; H 10.36%; O 5.87%

>>Variant: 5 α -form

CAS Registry Number: 14935-81-0

Molecular Formula: C₁₉H₂₈O

Molecular Weight: 272.43

Accurate Mass: 272.214015

Percentage Composition: C 83.77%; H 10.36%; O 5.87%

Physical Description: Cryst. (hexane)

Melting Point: Mp 125-126°

Optical Rotation: [α]_D +141 (CHCl₃)

>>Variant: 5 β -form

Molecular Formula: C₁₉H₂₈O

Molecular Weight: 272.43

Accurate Mass: 272.214015

Percentage Composition: C 83.77%; H 10.36%; O 5.87%

>>Derivative: 3 β ,4 β -Epoxide

Synonym(s): 3 β ,4 β -Epoxy-5 β -androstan-17-one

CAS Registry Number: 192192-77-1

Molecular Formula: C₁₉H₂₈O₂

Molecular Weight: 288.429

Accurate Mass: 288.20893

Percentage Composition: C 79.12%; H 9.78%; O 11.09%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 125-127°

References:

McKenna, J. *et al.*, *J.C.S.*, 1959, 2502, (*synth*)

Caglioti, L. *et al.*, *Tetrahedron*, 1964, **20**, 957, (*synth*)

Ihara, M. *et al.*, *J.C.S. Perkin I*, 1986, 117, (*synth*)

Andrade, L.C.R. *et al.*, *Acta Cryst. C*, 1997, **53**, 938-940, (*synth, cryst struct, epoxide*)