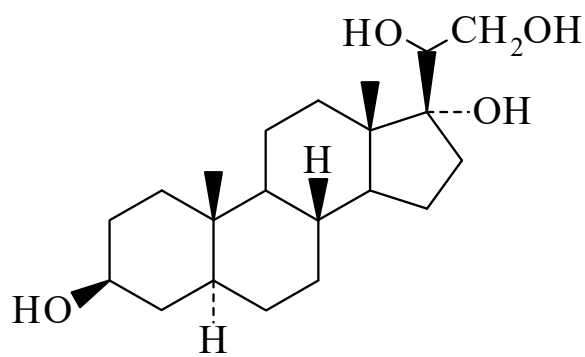




>>Entry Name: Pregnane-3,17,20,21-tetrol



Molecular Formula: C₂₁H₃₆O₄

Molecular Weight: 352.513

Accurate Mass: 352.26136

Percentage Composition: C 71.55%; H 10.29%; O 18.15%

>>Variant: (3β,5α,17αOH,20R)-form

Synonym(s): Reichstein's Substance K

CAS Registry Number: 566-41-6

Molecular Formula: C₂₁H₃₆O₄

Molecular Weight: 352.513

Accurate Mass: 352.26136

Percentage Composition: C 71.55%; H 10.29%; O 18.15%

Biological Source: Occurs in adrenal cortex

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 198-200°

Optical Rotation: $[\alpha]_D^{21} -1$ (c, 1.0 in EtOH)

>>Derivative: Tri-Ac

Molecular Formula: C₂₇H₄₂O₇

Molecular Weight: 478.625

Accurate Mass: 478.293055

Percentage Composition: C 67.76%; H 8.84%; O 23.40%

Physical Description: Cryst. (Et₂O/pentane)

Melting Point: Mp 179°

Optical Rotation: $[\alpha]_D^{19} +53.2$ (c, 1.9 in Me₂CO)

References:

Steiger, M. *et al.*, *Helv. Chim. Acta*, 1938, **21**, 546, (*synth*)

Serini, A. *et al.*, *Ber.*, 1939, **72**, 391, (*synth*)

Wagner, R.B. *et al.*, *J.A.C.S.*, 1950, **72**, 5301, (*synth*)