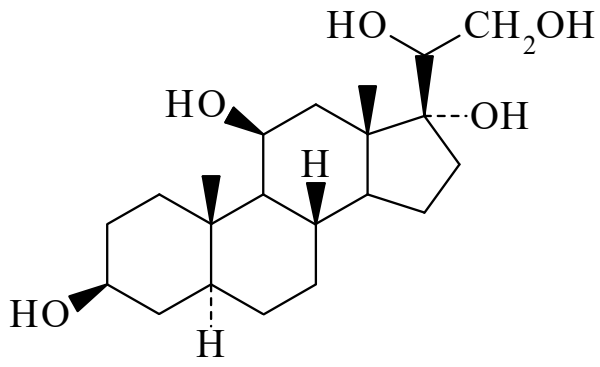
>>**Entry Name: Pregnane-3,11,17,20,21-pentol**



Molecular Formula: $C_{21}H_{36}O_5$
Molecular Weight: 368.512
Accurate Mass: 368.256275
Percentage Composition: C 68.45%; H 9.85%; O 21.71%

>>**Variant:** (3β,5α,11β,17αOH,20*R*)-form
Synonym(s): Reichstein's Substance A

CAS Registry Number: 516-39-2

Molecular Formula: $C_{21}H_{36}O_5$
Molecular Weight: 368.512
Accurate Mass: 368.256275
Percentage Composition: C 68.45%; H 9.85%; O 21.71%
Biological Source: Isol. from adrenal cortex
Use/Importance: Physiologically inactive
Physical Description: Cryst. (MeOH)
Melting Point: Mp 222°
Optical Rotation: $[\alpha]_D^{22}$+9.8 (c, 0.56 in MeOH)
Sigma: P9765

>>**Derivative:** Tri-Ac

Molecular Formula: $C_{27}H_{42}O_8$
Molecular Weight: 494.624
Accurate Mass: 494.28797
Percentage Composition: C 65.56%; H 8.56%; O 25.88%
Melting Point: Mp 220°
Optical Rotation: $[\alpha]_D$ +74 ($CHCl_3$)

>>**Variant:** (3α,5β,11β,17αOH,20*R*)-form

Molecular Formula: $C_{21}H_{36}O_5$
Molecular Weight: 368.512
Accurate Mass: 368.256275
Percentage Composition: C 68.45%; H 9.85%; O 21.71%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 266-269°

References:

Reichstein, T. *et al.*, *Helv. Chim. Acta*, 1941, **24**, 247E, *(isol)*
Sarett, L.H. *et al.*, *J.A.C.S.*, 1951, **73**, 1777, *(synth)*
Djerassi, C. *et al.*, *J. Biol. Chem.*, 1952, **194**, 115, *(synth)*
Ohrt, J.M. *et al.*, *Acta Cryst.*, 1965, **19**, 869, *(cryst struct)*

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