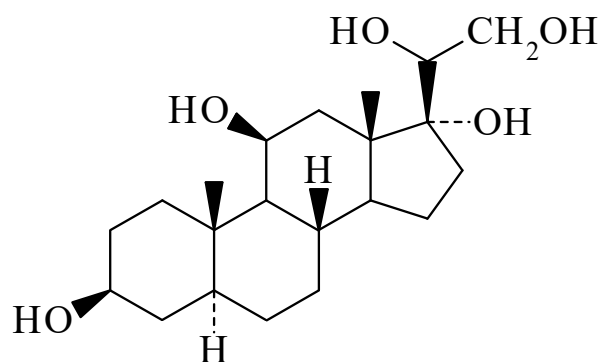




>>Entry Name: Pregnane-3,11,17,20,21-pentol



Molecular Formula: C₂₁H₃₆O₅

Molecular Weight: 368.512

Accurate Mass: 368.256275

Percentage Composition: C 68.45%; H 9.85%; O 21.71%

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

Synonym(s): Reichstein's Substance A

CAS Registry Number: 516-39-2

Molecular Formula: C₂₁H₃₆O₅

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: [α]_D²²+9.8 (c, 0.56 in MeOH)

Sigma: P9765

>>**Derivative:** Tri-Ac

Molecular Formula: C₂₇H₄₂O₈

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: [α]_D+74 (CHCl₃)

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

Molecular Formula: C₂₁H₃₆O₅

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*)