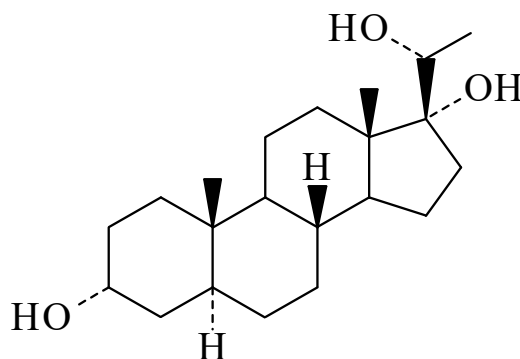




>>Entry Name: Pregnane-3,17,20-triol, 9CI



Extra CAS Registry Numbers(s): 27178-64-9

Molecular Formula: C₂₁H₃₆O₃

Molecular Weight: 336.514

Accurate Mass: 336.266445

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

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

Synonym(s): (3 α ,5 α ,17 α OH,20 β)-form

CAS Registry Number: 13933-75-0

Molecular Formula: C₂₁H₃₆O₃

Molecular Weight: 336.514

Accurate Mass: 336.266445

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 226-229°

Optical Rotation: [α]_D²⁵ -5.8 (CHCl₃)

Sigma: P2507

>>Variant: (3 α ,5 α ,17 α OH,20*S*)-form

Synonym(s): (3 α ,5 α ,17 α OH,20 α)-form

CAS Registry Number: 16134-59-1

Molecular Formula: C₂₁H₃₆O₃

Molecular Weight: 336.514

Accurate Mass: 336.266445

Percentage Composition: C 74.95%; H 10.78%; O 14.26%

Melting Point: Mp 228-230°

Optical Rotation: [α]_D²⁶ -13.2 (CHCl₃)

>>Derivative: 20-Ac

Molecular Formula: C₂₃H₃₈O₄

Molecular Weight: 378.551

Accurate Mass: 378.27701

Percentage Composition: C 72.98%; H 10.12%; O 16.91%

Physical Description: Cryst. (Me₂CO/petrol)

Melting Point: Mp 213-216.5°

Optical Rotation: [α]_D²⁸ -20.7 (CHCl₃)

>>Derivative: 3,20-Di-Ac

Molecular Formula: C₂₅H₄₀O₅

Molecular Weight: 420.588

Accurate Mass: 420.287575

Percentage Composition: C 71.39%; H 9.59%; O 19.02%

Melting Point: Mp 123-124 and 130-131° (double Mp)

Optical Rotation: [α]_D²² -15.7 (CHCl₃)