



>>Entry Name: 20-Hydroxypregnan-3-one, 9Cl

Related CAS Registry Numbers(s): 22215-65-2 22215-66-3 23885-50-9 23885-51-0

Molecular Formula: C₂₁H₃₄O₂

Molecular Weight: 318.498

Accurate Mass: 318.25588

Percentage Composition: C 79.19%; H 10.76%; O 10.05%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 128-129°

>>Variant: (5 α ,20*R*)-form

CAS Registry Number: 516-58-5

Molecular Formula: C₂₁H₃₄O₂

Molecular Weight: 318.498

Accurate Mass: 318.25588

Percentage Composition: C 79.19%; H 10.76%; O 10.05%

Physical Description: Cryst. (heptane)

Melting Point: Mp 189-190°

Optical Rotation: [α]_D +20 (c, 1.2 in CHCl₃)

>>Derivative: Ac

Molecular Formula: C₂₃H₃₆O₃

Molecular Weight: 360.536

Accurate Mass: 360.266445

Percentage Composition: C 76.62%; H 10.06%; O 13.31%

Physical Description: Cryst. (heptane)

Melting Point: Mp 148-149°

Optical Rotation: [α]_D +57 (c, 1.9 in CHCl₃)

>>Derivative: Oxime

Molecular Formula: C₂₁H₃₅NO₂

Molecular Weight: 333.513

Accurate Mass: 333.266779

Percentage Composition: C 75.63%; H 10.58%; N 4.20%; O 9.59%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 216°

>>Variant: (5 α ,20*S*)-form

CAS Registry Number: 516-59-6

Molecular Formula: C₂₁H₃₄O₂

Molecular Weight: 318.498

Accurate Mass: 318.25588

Percentage Composition: C 79.19%; H 10.76%; O 10.05%

Physical Description: Cryst. (Me₂CO aq)

Melting Point: Mp 179°

Optical Rotation: [α]_D +36.6 (c, 0.8 in CHCl₃)

Sigma: P6413

>>Derivative: Ac

Physical Description: Cryst. (EtOH)

Melting Point: Mp 161-162°

Optical Rotation: [α]_D +24 (c, 1.5 in CHCl₃)