



>>Entry Name: Pregna-4,6-diene-3,20-dione, 9CI

Synonym(s): 6,7-Didehydropregesterone

CAS Registry Number: 1162-56-7

Molecular Formula: $C_{21}H_{28}O_2$

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Source/Synthesis: Synth. steroid prod. by the modified Oppenauer oxidn. of pregnenolone using quinone as the hydrogen acceptor

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 147-148°

Optical Rotation: $[\alpha]_D +167$ (CHCl₃)

Other Data: About one third as active as progesterone

>>Variant: 17 α -form

CAS Registry Number: 25093-47-4

Molecular Formula: $C_{21}H_{28}O_2$

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Physical Description: Needles (C₆H₆/hexane)

Melting Point: Mp 150-151°

Optical Rotation: $[\alpha]_D^{28} -80$ (CHCl₃)

>>Variant: (8 α ,10 α)-form

Molecular Formula: $C_{21}H_{28}O_2$

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 119-121 and 130-131° (double Mp)

Optical Rotation: $[\alpha]_D^{22} +200$ (CHCl₃)

>>Variant: 9 β -form

Molecular Formula: $C_{21}H_{28}O_2$

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 163-164°

Optical Rotation: $[\alpha]_D +256$ (c, 0.22 in CHCl₃)

>>Variant: (9 β ,10 α)-form

Molecular Formula: $C_{21}H_{28}O_2$

Molecular Weight: 312.451

Accurate Mass: 312.20893

Percentage Composition: C 80.73%; H 9.03%; O 10.24%

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 169-170°

Optical Rotation: $[\alpha]_D^{25} -484.5$ (CHCl₃)

>>Derivative: Dioxime

Physical Description: Cryst. (THF/petrol)

Melting Point: Mp 279-282°

References: