



>>Entry Name: 16,17-Epoxy pregn-4-ene-3,20-dione
ENTRY UNDER REVIEW

Molecular Formula: C₂₁H₂₈O₃
Molecular Weight: 328.45
Accurate Mass: 328.203845
Percentage Composition: C 76.79%; H 8.59%; O 14.61%

>>Variant: 16 α -form
Synonym(s): 16 α ,17 α -Epoxyprogesterone

CAS Registry Number: 1097-51-4

Molecular Formula: C₂₁H₂₈O₃
Molecular Weight: 328.45
Accurate Mass: 328.203845
Percentage Composition: C 76.79%; H 8.59%; O 14.61%
Physical Description: Cryst. (MeOH)
Melting Point: Mp 211°
Optical Rotation: [α]_D +167 (CHCl₃)

Sigma: E5125

>>Variant: 16 β -form

CAS Registry Number: 16356-47-1
Molecular Formula: C₂₁H₂₈O₃
Molecular Weight: 328.45
Accurate Mass: 328.203845
Percentage Composition: C 76.79%; H 8.59%; O 14.61%
Physical Description: Cryst. (Me₂CO/hexane)
Melting Point: Mp 148-149°
Optical Rotation: [α]_D²⁵ +69 (CHCl₃)

References:

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Yang, N.C. *et al.*, *J.A.C.S.*, 1958, **80**, 5845, (*synth*)
Berg, R.G., *J.O.C.*, 1962, **27**, 3350, (*synth*)
Tori, K. *et al.*, *J.O.C.*, 1964, **29**, 1136, (*pmr*)
Toft, P. *et al.*, *Can. J. Pharm. Sci.*, 1972, **7**, 53, (*ms*)
Hofmeister, H. *et al.*, *Chem. Ber.*, 1976, **109**, 185
Goubitz, K. *et al.*, *Steroids*, 1984, **44**, 153, (*cryst struct*)