



>>Entry Name: Pregnane-3,11,20-trione

ENTRY UNDER REVIEW

CAS Registry Number: 16052-29-2

Related CAS Registry Numbers(s): 72205-32-4 72205-34-6 83014-66-8

Molecular Formula: C₂₁H₃₀O₃

Molecular Weight: 330.466

Accurate Mass: 330.219495

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

>>Variant: 5 α -form

CAS Registry Number: 2089-06-7

Molecular Formula: C₂₁H₃₀O₃

Molecular Weight: 330.466

Accurate Mass: 330.219495

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 211-213°

Optical Rotation: [α]_D +133 (EtOH)

Sigma: P3421

>>Variant: 5 β -form

CAS Registry Number: 1474-68-6

Molecular Formula: C₂₁H₃₀O₃

Molecular Weight: 330.466

Accurate Mass: 330.219495

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 155-158°

Optical Rotation: [α]_D +122 (EtOH)

>>Variant: (5 α ,14 β ,17 α)-form

CAS Registry Number: 53176-89-9

Molecular Formula: C₂₁H₃₀O₃

Molecular Weight: 330.466

Accurate Mass: 330.219495

Percentage Composition: C 76.33%; H 9.15%; O 14.52%

Physical Description: Cryst.

Melting Point: Mp 155°

Optical Rotation: [α]_D +43 (c, 0.37 in CH₂Cl₂)

>>Derivative: 3,20-Bis(cyclic 1,2-ethylene acetal)

CAS Registry Number: 53176-90-2

Physical Description: Cryst.

Melting Point: Mp 152°

Optical Rotation: [α]_D +50 (c, 0.46 in CH₂Cl₂)

References:

- Djerassi, C. *et al.*, *J.A.C.S.*, 1953, **75**, 3505, (*synth*)
Schmitt, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1964, 753, (*synth*)
Nussim, C. *et al.*, *J.O.C.*, 1964, **29**, 1120, (*synth*)
Greenspan, G. *et al.*, *J.O.C.*, 1965, **30**, 4215, (*synth*)
Shoppee, C.W. *et al.*, *Tetrahedron, Suppl. No. 8*, 1966, 421, (*pmr, ms*)
Obermann, H. *et al.*, *Chem. Ber.*, 1970, **103**, 1497, (*ms*)
Gough, J.L. *et al.*, *Chem. Comm.*, 1972, 979, (*cmr*)
Gull, P. *et al.*, *Helv. Chim. Acta*, 1974, **57**, 863, (5 α ,14 β ,17 α -form)
Ikegawa, S. *et al.*, *Chem. Pharm. Bull.*, 1979, **27**, 1864, (*synth*)