



>>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: $C_{21}H_{30}O_3$

Molecular Weight: 330.466

Accurate Mass: 330.219495

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

>>Variant: 5α -form

CAS Registry Number: 2089-06-7

Molecular Formula: $C_{21}H_{30}O_3$

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: $[\alpha]_D +133$ (EtOH)

Sigma: P3421

>>Variant: 5β -form

CAS Registry Number: 1474-68-6

Molecular Formula: $C_{21}H_{30}O_3$

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: $[\alpha]_D +122$ (EtOH)

>>Variant: ($5\alpha,14\beta,17\alpha$)-form

CAS Registry Number: 53176-89-9

Molecular Formula: $C_{21}H_{30}O_3$

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: $[\alpha]_D +43$ (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: $[\alpha]_D +50$ (c, 0.46 in CH₂Cl₂)

References:

- Djerassi, C. *et al.*, *J.A.C.S.*, 1953, **75**, 3505, (*synth*)
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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, ($5\alpha,14\beta,17\alpha$ -form)
Ikegawa, S. *et al.*, *Chem. Pharm. Bull.*, 1979, **27**, 1864, (*synth*)