



Sigma: D6128
Supelco: R42-6680

>>Derivative: Ac

CAS Registry Number: 1255-88-5
Molecular Formula: $C_{29}H_{50}O_2$
Molecular Weight: 430.713
Accurate Mass: 430.38108
Percentage Composition: C 80.87%; H 11.70%; O 7.43%
Physical Description: Prisms (MeOH/EtOAc)
Melting Point: Mp 110-111°
Optical Rotation: $[\alpha]_D^{20} +11.5$ (CHCl₃)

>>Derivative: 3-O-Sulfate

Molecular Formula: $C_{27}H_{48}O_4S$
Molecular Weight: 468.74
Accurate Mass: 468.32733
Percentage Composition: C 69.18%; H 10.32%; O 13.65%; S 6.84%
Melting Point: Mp 174-175.5° (as Na salt)
Optical Rotation: $[\alpha]_D^{29} +16.6$ (EtOH) (as Na salt)

>>Variant: (3 α ,5 β)-form
Synonym(s): Epicoprostanol. Epicoprosterol

CAS Registry Number: 516-92-7

Molecular Formula: $C_{27}H_{48}O$
Molecular Weight: 388.676
Accurate Mass: 388.370515
Percentage Composition: C 83.44%; H 12.45%; O 4.12%
Biological Source: Found in ambergris and dog faeces
Melting Point: Mp 107-108°
Optical Rotation: $[\alpha]_D +31$ (CHCl₃)
Aldrich: 28539-0
Sigma: C2882
Supelco: R47-5100

>>Variant: (3 β ,5 β)-form
Synonym(s): Coprostanol. Coprosterol. Stercorin

CAS Registry Number: 360-68-9
Extra CAS Registry Numbers(s): 17608-41-2

Molecular Formula: $C_{27}H_{48}O$
Molecular Weight: 388.676
Accurate Mass: 388.370515
Percentage Composition: C 83.44%; H 12.45%; O 4.12%
Biological Source: Major sterol from faeces
Use/Importance: Used to monitor disposal of human excretion
Melting Point: Mp 96-100°
Optical Rotation: $[\alpha]_D +26$ (CHCl₃)
Sigma: C7578

>>Derivative: Ac

Molecular Formula: $C_{29}H_{50}O_2$
Molecular Weight: 430.713
Accurate Mass: 430.38108
Percentage Composition: C 80.87%; H 11.70%; O 7.43%
Melting Point: Mp 89°

References: