



Formula: C₂₁H₃₄O₂

MW: 318.5

CAS: 516-54-1

Smiles:

C1[C]2([C@H]([C@@H]3(CC[C@@H]4([C]([C@@H]3(C1)))(CC[C@H](O)C4)C)))(CC[C@@H]2C(=O)C)C

THERAPEUTIC CATEGORY: Anesthetic (local)

SOURCE: Naturally occurring metabolite of progesterone

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 0

N+O: 2

Chiral Centers: 8

LogP: 6.49

LogS: -5.47

LIPINSKI: 3

Synonyms:

3-alpha,5-alpha-pregnanolone;3-alpha,5-alpha-tetrahydroprogesterone;3-alpha-hydroxy-5-alpha-pregnan-20-one;5alpha-Pregnan-20-one, 3alpha-hydroxy-;allotetrahydroprogesterone;Pregnan-20-one, 3-hydroxy-, (3alpha,5alpha)-;5ALPHA-PREGNAN-3ALPHA-OL-20-ONE;3ALPHA-HYDROXY-5ALPHA-20-ONE

CAS:516-54-1

MF:C21H34O2

MW:318.49

EINECS:

Product Categories: ALLOPREGNAN-3ALPHA-OL-20-ONE

Chemical Properties: storage temp. Store at RT solubility chloroform: 20 mg/mL, clear, colorless Merck 13,272

CAS DataBase Reference: 516-54-1(

CAS DataBase Reference:)

Safety Information: Safety Statements 22-24/25 WGK Germany 3 RTECS TU4383000 F 10 ALLOPREGNAN-3ALPHA-OL-20-ONE

Usage And Synthesis: Biological ActivityGABA A receptor positive allosteric modulator. Neuroactive steroid. ALLOPREGNAN-3ALPHA-OL-20-ONE

