



Formula: C₂₇H₄₀O₄

MW: 428.61

CAS: 630-56-8

TNP NUMBER: TNP00609

MDL NUMBER: MFCD03225569

IUPAC: (1S,11S,15S,2R,10R,14R)-14-acetyl-2,15-dimethyl-5-oxotetracyclo[8.7.0.0.0]heptadec-6-en-14-yl hexanoate

Smiles:

O(CCCCCC=O)[C@@]1(C(C)=O)[C@]2(C)[C@@H](CC1)([C@H]1([C@H](CC2)([C@]2(C)C(CC1)=CC(CC2)=O)))

Medical use is similar to that of progesterone; causes virilizing changes in a female fetus

THERAPEUTIC CATEGORY: Progestogen

ACCEPTORS: 4

DONORS: 0

ROTATION BONDS: 6

N+O: 4

Chiral Centers: 6

LogP: 7.51

LogS: -6.37

LIPINSKI: 3

Synonyms: PREGN-4-ENE-3,20-DIONE
HEXANOATE;17-((1-oxohexyl)oxy)-pregn-4-ene-20-dione;17-((1-Oxohexyl)oxy)pregn-4-ene-3,20-dione;17a-hydroxyprogesteronehexanoate;17-alpha-Hexanoyloxypregn-4-ene-3,20-dione;17alpha-Hydroxyprogesterone
n-caproate;17-alpha-hydroxyprogesteronen-caproate;17-Hydroxypregn-4-ene-3,20-dione
caproate

CAS:630-56-8

MF:C27H40O4

MW:428.6

EINECS:211-138-8

Product Categories:Biochemistry;Hydroxyketosteroids;Steroids 17a-Hydroxyprogesterone
caproate

Chemical Properties: mp 119C Merck 4839

CAS DataBase Reference: 630-56-8(

CAS DataBase Reference:) NIST Chemistry ReferenceIsoquinolinedione, 1,3(2h,4h)-,
2-hydroxy, acetate ester(630-56-8) EPA Substance Registry SystemPregn-4-ene-3,20- dione,
17-[(1-oxohexyl)oxy]-(630-56-8) T Risk Statements 61 Safety Statements 53-22-36/37/39-45
WGK Germany 3 RTECS TU5085000 17a-Hydroxyprogesterone caproate

Usage And Synthesis: 17a-Hydroxyprogesterone caproate

