



Formula: C₂₁H₃₀O₅

MW: 362.47

CAS: 50-23-7

MDL: MFCD01533852

TNP: TNP00371

11,17a,21-Trihydroxy-4-pragnene-3,20-dione; 11-beta,17,21-trihydroxypregn-4-ene-3,20-dione;
11beta,17,21-Trihydroxypregn-4-ene-3,20-dione;
11-beta,17-alpha,21-trihydroxy-4-pregnene-3,20-dione;
11beta,17alpha,21-Trihydroxy-4-pregnene-3,20-dione; 11-beta,17-alph



LogP: 1.61

LogS:

Acceptors: 5

Donors: 3

Rotation Bonds: 3

Chiral Centers: 7

N+O: 5

LIPINSKY: 4

IUPAC: (1S,10S,11S,15S,17S,2R,14R)-14,17-dihydroxy-14-(2-hydroxyacetyl)-2,15-dimethyl tetracyclo[8.7.0.0.0]heptadec-6-en-5-one

Smiles:

C=12[C]([C@H]3([C@H](C[C]4([C](C(=O)CO)(CC[C@@H]4([C@@H]3(CC2)))O)C)O))(CCC(=

O)C1)C

Specification: TPI; Steroids; Veterinaries Hydrocortisone Chemical Properties:

mp 211-214 C(lit.) alpha 166