



Formula: C<sub>24</sub>H<sub>31</sub>FO<sub>6</sub>

MW: 434.5

CAS: 1177-87-3

TNP NUMBER: TNP00599

MDL NUMBER: MFCD03548192

IUPAC: 2-((2S,10S,11S,15S,17S,1R,13R,14R)-1-fluoro-14,17-dihydroxy-2,13,15-trimethyl-5-oxotetracyclo[8.7.0.0.0]heptadeca-3,6-dien-14-yl)-2-oxoethyl acetate

Smiles:

C=12[C]([C]3([C@H](C[C]4([C@H]([C@@H]3(CC2)))(C[C@H]([C]4(C(COC(=O)C)=O)O)C))C)O)F)(C=CC(=O)C1)C

Glucocorticoid; anti-inflammatory agent; diagnostic aid (Cushing's syndrome, depression)

THERAPEUTIC CATEGORY: Glucocorticoid; anti-inflammatory agent; diagnostic aid (Cushing's syndrome, depression)

ACCEPTORS: 6

DONORS: 2

ROTATION BONDS: 4

N+O: 6

Chiral Centers: 8

LogP: 3.52

LogS: -4.83

LIPINSKI: 4

Synonyms: DEXAMETHASON ACETATE;dexamethasone-17-acetate;DEXAMETHASONE 21-ACETATE;DEXAMETHASONE ACETATE;9ALPHA-FLUORO-16ALPHA-METHYL-11BETA,17ALPHA,21-TRIHYDROXY-1,4-P REGNADIENE-3,20-DIONE-21-ACETATE;9-ALPHA-FLUORO-16-ALPHA-METHYL-11-BETA,1 7-ALPHA,21-TRIHYDROXY-1,4-PREGNADIENE-3,20-DIONE ACETATE;9ALPHA-FLUORO-16ALPHA-METHYLPREDNISOLONE-21-ACETATE;9 ALPHA-FLUORO-11 BETA,17 ALPHA,21-TRIHYDRO-16 ALPHA-METHYLPREGNA-1,4-DIENE-3,20-DIONE-21-ACETATE

CAS:1177-87-3

MF:C24H31FO6

MW:434.5

EINECS:214-646-8

Product Categories:Biochemistry;Hydroxyketosteroids;Steroids Dexamethasone-17-acetate

Chemical Properties: mp 238-240 C(lit.) refractive index 87 (C=1, Dioxane) storage temp. 2-8C Merck 2943

CAS DataBase Reference: 1177-87-3(

CAS DataBase Reference: ) NIST Chemistry ReferencePrednisolone, 9alpha-fluoro-16alpha-methyl-, acetate(1177-87-3) EPA Substance Registry SystemPregna-1,4-diene- 3,20-dione, 21-(acetyloxy)-9-fluoro-11, 17-dihydroxy-16-methyl-, (11.beta.,16.alpha.)-(1177-87-3) Xi Risk Statements 43 Safety Statements 36/37 WGK Germany 3 RTECS TU4050000 Dexamethasone-17-acetate

Usage And Synthesis: Dexamethasone-17-acetate

