Prednisolone Acetate

Other names:
(11«beta»)-21-(Acetyloxy)-11,17-dihydroxypregna-1,4-diene-3,20-dione
(11Â«betaÂ»)-21-(Acetyloxy)-11,17-dihydroxypregna-1,4-diene-3,20-dione
1,4-Pregnadiene-3,20-dione, 11beta,17alpha,21-trihydroxy-, 21-acetate
1,4-Pregnadiene-3,20-dione, 11beta,17alpha,21-trihydroxy-, acetate
11«beta»,17«alpha»,21-Trihydroxypregna-1,4-diene-3,20-dione 21-acetate
11Â«betaÂ»,17Â«alphaÂ»,21-Trihydroxypregna-1,4-diene-3,20-dione 21-acetate
Ak-Tate
Cormalone
Cortipred
Delcort-E
Deltilen
Durapred
Econopred
Hydroprednisone acetate
Inflanefran
Meticortelone acetate
Meticotelone acetate
NSC 10966
Nisolone
Pred Forte
Pred Forte TM
Pred Mild
Predalone 50
Prediacortine
Predicort
Prednelan-N
Prednidoren
Prednisolone 21-acetate
Predonine injection
Pregna-1,4-diene-3,20-dione, 11«beta»,17,21-trihydroxy-, 21-acetate
Pregna-1,4-diene-3,20-dione, 11Â«betaÂ»,17,21-trihydroxy-, 21-acetate
Pregna-1,4-diene-3,20-dione, 21-(acetyloxy)-11,17-dihydroxy-, (11«beta»)-
Pregna-1,4-diene-3,20-dione, 21-(acetyloxy)-11,17-dihydroxy-, (11Â«betaÂ»)-
Prenema
Pricortin
Sterane
Supercortyl

Inchi: InChI=1S/C23H30O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14

InchiKey: LRJOMUJRLNCICJ-RJNDBBCYSA-N

Formula: C23H30O6

SMILES: CC(=O)OCC(=O)C1(O)CCC2C3CCC4=CC(=O)C=CC4(C)C3C(O)CC21C
Mol. weight [g/mol]: 402.48
CAS: 52-21-1

Physical Properties

Property code	Value	Unit	Source
gf	-423.10	kJ/mol	Joback Method
hf	-968.40	kJ/mol	Joback Method
hfus	35.81	kJ/mol	Joback Method
hvap	117.68	kJ/mol	Joback Method
log10ws	-4.37		Estimated Solubility Method
log10ws	-4.37		Aqueous Solubility Prediction Method
logp	2.128		Crippen Method
mcvol	305.210	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
tb	1146.30	K	Joback Method
tc	1403.40	K	Joback Method
tf	788.10	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.90	J/mol×K	1146.30	Joback Method
cpg	1319.57	J/mol×K	1189.15	Joback Method
cpg	1369.55	J/mol×K	1232.00	Joback Method
cpg	1424.36	J/mol×K	1274.85	Joback Method
cpg	1484.55	J/mol×K	1317.70	Joback Method
cpg	1550.66	J/mol×K	1360.55	Joback Method
cpg	1623.21	J/mol×K	1403.40	Joback Method
hfust	42.30	kJ/mol	515.00	NIST Webbook
hfust	38.67	kJ/mol	511.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume