Hydrocortisone acetate

Other names:

11,17-Dihydroxy-3,20-dioxopregn-4-en-21-yl acetate, (11«beta»)-
11«beta»,17«alpha»,21-Trihydroxypregn-4-ene-3,20-dione 21-acetate
11«beta»,17«alpha»-Dihydroxy-21-acetoxypregesterone
17-Hydroxycorticosterone acetate
17-Hydroxycorticosterone-21-acetate
17«alpha»-Hydrocorticosterone-21-acetate
17«alpha»-Hydroxycorticosterone acetate
21-Acetoxy-11«beta»,17-dihydroxypregn-4-en-3,20-dione
21-Acetoxy-11«beta»,17-dihydroxypregn-4-ene-3,20-dione
21-Acetoxy-11«beta»,17«alpha»-dihydroxypregn-4-ene-3,20-dione
Abbocort
Acetate-AS
Aceto-Cort
Anusol-HC
Bambicort
Berlison F
Biocortar
CaldeCort
Carmol HC
Chemysone
Colifoam
Collusul-HC
Colofoam
Compound F acetate
Cordes
Cortacream
Cortaid
Cortef acetate
Cortell
Cortes
Corticosterone, 17-hydroxy-, 21-acetate
Cortifoam
Cortisol acetate
Cortisol, 21-acetate
Cortril acetate
Cortril acetate-AS
Efcolin
Eye-Cort
Fernisone
HA

Hc45
Hycortole acetate
Hydrin-2
Hydrocal
Hydrocortisat
Hydrocortisone 21-acetate
Hydrocortistab
Hydrocortone acetate
Hydrosone
Hydroxycorticosterone acetate
Hysone-A
Isopto-Hydrocortisone
Lanacort
Lenirit
Mysone
NSC 741
Pabracort
Pregn-4-ene-3,20-dione, 11«beta»,17,21-trihydroxy-, 21-acetate
Pregn-4-ene-3,20-dione, 21-(acetoxy)-11,17-dihydroxy-, (11-«beta»)-
Pregn-4-ene-3,20-dione, 21-(acetyloxy)-11,17-dihydroxy-, (11«beta»)-
Proctocort
Resicort
Sigmacort
Sintotrat
Velopural
Wycort

Inchi: InChI=1S/C23H32O6/c1-13(24)29-12-19(27)23(28)9-7-17-16-5-4-14-10-15(25)6-8-21(14

InchiKey: ALEXXDVDDISNDU-MCHRFJOXSA-N

Formula: C23H32O6

SMILES: CC(=O)OCC(=O)[C@@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3[C

Mol. weight [g/mol]: 404.50

Physical Properties

Property code	Value	Unit	Source
hfus	34.59	kJ/mol	Joback Method
log10ws	-4.30		Aqueous Solubility Prediction Method
log10ws	-4.88		Estimated Solubility Method
logp	2.352		Crippen Method

mcvol	309.510	ml/mol	McGowan Method
tf	472.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.14	J/mol×K	1147.14	Joback Method
cpg	1354.32	J/mol×K	1190.02	Joback Method
cpg	1404.71	J/mol×K	1232.90	Joback Method
cpg	1459.86	J/mol×K	1275.78	Joback Method
cpg	1520.29	J/mol×K	1318.67	Joback Method
cpg	1586.56	J/mol×K	1361.55	Joback Method
cpg	1659.18	J/mol×K	1404.43	Joback Method
hfust	53.64	kJ/mol	480.00	NIST Webbook
hfust	36.95	kJ/mol	496.00	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50033&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point