

Prednisolone

Other names:

.DELTA.1-cortisol
.DELTA.1-dehydrocortisol
.DELTA.1-dehydrohydrocortisone
.DELTA.1-hydrocortisone
1,2-Dehydrohydrocortisone
1,4-Pregnadien-11-«beta»,17-«alpha»,21-triol-3,20-dione
1,4-Pregnadien-11-Â«betaÂ»,17-Â«alphaÂ»,21-triol-3,20-dione
1,4-Pregnadiene-11-«beta»,17-«alpha»,21-triol-3,20-dione
1,4-Pregnadiene-11-Â«betaÂ»,17-Â«alphaÂ»,21-triol-3,20-dione
1,4-Pregnadiene-3,20-dione-11-«beta»,17-«alpha»,21-triol
1,4-Pregnadiene-3,20-dione-11-Â«betaÂ»,17-Â«alphaÂ»,21-triol
1,4-pregnadiene-11.beta.,17.alpha.,21-triol-3,20-dione
1-Dehydrohydrocortisone
11,17,21-Trihydroxypregna-1,4-diene-3,20-dione, (11«beta»)-
11,17,21-Trihydroxypregna-1,4-diene-3,20-dione, (11Â«betaÂ»)-
11-«beta»,17,21-Trihydroxypregna-1,4-diene-3,20-dione
11-«beta»,17-«alpha»,21-Trihydroxy-1,4-pregnadiene-3,20-dione
11-«beta»,17-«alpha»,21-Trihydroxypregna-1,4-diene-3,20-dione
11-Â«betaÂ»,17,21-Trihydroxypregna-1,4-diene-3,20-dione
11-Â«betaÂ»,17-Â«alphaÂ»,21-Trihydroxy-1,4-pregnadiene-3,20-dione
11-Â«betaÂ»,17-Â«alphaÂ»,21-Trihydroxypregna-1,4-diene-3,20-dione
11.beta.,17.alpha.,21-trihydroxypregna-1,4-diene-3,20-dione
Co-Hydeltra
Codelcortone
Cordrol
Cortalone
Cotogesic
Decaprednil
Decortin H
Delcortol
Delta F
Delta-Cortef
Delta-Ef-Cortelan
Delta-Stab
Deltacortenol
Deltacortril
Deltahydrocortisone
Deltasolone
Deltisolone
Derpo PD

Dexa-Cortidelt Hostacortin H
Di-Adreson F
Dicortol
Donisolone
Dydeltrone
Eazolin D
Erbacort
Erbasona
Estilsona
Fernisolone
Fernisolone P
Hostacortin
Hostacortin H
Hydeltra
Hydeltrone
Hydrodeltalone
Hydrodeltisone
Hydroretrocortin
Hydroretrocortine
K 1557
Klismacort
Lentosone
Metacortandralone
Meti-Derm
Meticortelone
PRDL
Panafcortelone
Paracortol
Paracotol
Precortancyl
Precortilon
Precortisyl
Predne-Dome
Prednelan
Prednicen
Predniliderm
Prednis
Predonin
Predonine
Preflam
Pregna-1,4-diene-3,20-dione, 11,17,21-trihydroxy-, (11«beta»)-
Pregna-1,4-diene-3,20-dione, 11,17,21-trihydroxy-, (11Â«betaÂ»)-
Pregna-1,4-diene-3,20-dione, 11«beta»,17,21-trihydroxy-

Pregna-1,4-diene-3,20-dione, 11Â«betaÂ»,17,21-trihydroxy-
Prelone
Prenolone
Rolisone
Scherisolon
Solone
Steran
Sterane
Sterolone
Ulacort
Ultracorten H
Ultracortene-H
Ultracortene-hydrogen
pregna-1,4-diene-3,20-dione, 11,17,21-trihydroxy-, (11.beta.)-
pregna-1,4-diene-3,20-dione, 11.beta.,17,21-trihydroxy-
«DELTA»1-Cortisol
«DELTA»1-Dehydrocortisol
«DELTA»1-Dehydrohydrocortisone
«DELTA»1-Hydrocortisone
Â«DELTAÂ»1-Cortisol
Â«DELTAÂ»1-Dehydrocortisol
Â«DELTAÂ»1-Dehydrohydrocortisone
Â«DELTAÂ»1-Hydrocortisone

Inchi: InChI=1S/C21H28O5/c1-19-7-5-13(23)9-12(19)3-4-14-15-6-8-21(26,17(25)11-22)20(15,2
InchiKey: OIGNJSKKLXVSLS-NDNUHCHRSA-N
Formula: C21H28O5
SMILES: CC12C=CC(=O)C=C1CCC1C2C(O)CC2(C)C1CCC2(O)C(=O)CO
Mol. weight [g/mol]: 360.44
CAS: 50-24-8

Physical Properties

Property code	Value	Unit	Source
gf	-342.84	kJ/mol	Joback Method
hf	-834.55	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hvap	120.75	kJ/mol	Joback Method
log10ws	-3.18		Estimated Solubility Method
log10ws	-3.15		Aqueous Solubility Prediction Method

logp	1.558		Crippen Method
mccvol	275.460	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
tb	1116.43	K	Joback Method
tc	1366.85	K	Joback Method
tf	511.48	K	Aqueous Solubility Prediction Method
vc	1.032	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.62	J/mol×K	1116.43	Joback Method
cpg	1193.94	J/mol×K	1158.17	Joback Method
cpg	1240.40	J/mol×K	1199.90	Joback Method
cpg	1291.52	J/mol×K	1241.64	Joback Method
cpg	1347.81	J/mol×K	1283.37	Joback Method
cpg	1409.79	J/mol×K	1325.11	Joback Method
cpg	1477.98	J/mol×K	1366.85	Joback Method
hfust	38.86	kJ/mol	513.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Bicalutamide, Megestrol Acetate, Prednisolone, Betamethasone, Hydrocortisone, and Prednisolone at Different Temperatures from 298.15 to 443.15 K:	https://www.doi.org/10.1021/acs.jced.6b00997
Joback Method:	https://www.doi.org/10.1021/je900376r
Aqueous Solubility Prediction Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt http://link.springer.com/article/10.1007/BF02311772

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

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