Prednisone

Other names:

Pregna-1,4-diene-3,11,20-trione, 17,21-dihydroxy-
«DELTA»-Cortisone
«DELTA»1-Dehydrocortisone
«DELTA»1-Cortisone
Delta-E
Ancortone
Bicortone
Colisone
Cortidelt
Dacortin
Decortancyl
Decortisyl
Dehydrocortisone
Dekortin
Delta-Cortelan
Deltacortisone
Deltacortone
Deltasone
Deltison
Deltisone
Deltra
Di-Adreson
Encorton
Encortone
Enkorton
Hostacortin
Metacortandracin
Meticorten
NSC 10023
Paracort
Prednison
Prednizon
Rectodelt
Supercortil
Ultracorten
Ultracortene
1-Dehydrocortisone
1,2-Dehydrocortisone
Cortan
Cotone

	Decortin
	Delta-Dome
	In-Sone
	Juvason
	Lisacort
	NCI-C04897
	Orasone
	Prednicen-M
	Prednilonga
	Servisone
	SK-Prednisone
	U 6020
	Wojtab
	Zenadrid
	1,4-Pregnadiene-17«alpha»,21-diol-3,11,20-trione
	17,21-Dihydroxypregna-1,4-diene-3,11,20-trione
	17«alpha»,21-Dihydroxy-1,4-pregnadiene-3,11,20-trione
	Adasone
	Cartancyl
	Deltisona
	Fernisone
	Panafcort
	Winpred
	Nurison
	Sterapred
Inchi:	InChI=1S/C21H26O5/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:	XOFYZVNMUHMLCC-NUBBXXJJSA-N
Formula:	C21H26O5
SMILES:	CC12C=CC(=O)C=C1CCC1C2C(=O)CC2(C)C1CCC2(O)C(=O)CO
Mol. weight [g/mol]:	358.43
CAS:	53-03-2

Physical Properties

Property code	Value	Unit	Source
gf	-320.90	kJ/mol	Joback Method
hf	-799.68	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	108.62	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method

logp	1.766		Crippen Method
mcvol	271.160	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	2651.00		NIST Webbook
tb	1096.74	K	Joback Method
tc	1347.58	K	Joback Method
tf	765.86	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.96	J/mol×K	1096.74	Joback Method
cpg	1142.88	J/mol×K	1138.55	Joback Method
cpg	1185.34	J/mol×K	1180.35	Joback Method
cpg	1231.82	J/mol×K	1222.16	Joback Method
cpg	1282.80	J/mol×K	1263.97	Joback Method
cpg	1338.77	J/mol×K	1305.77	Joback Method
cpg	1400.20	J/mol×K	1347.58	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53032&Units=SI

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume