Corticosterone

Other names:	(11«beta»)-11,21-Dihydroxypregn-4-ene-3,20-dione
	(11Â«betaÂ»)-11,21-Dihydroxypregn-4-ene-3,20-dione
	11,21-Dihydroxyprogesterone
	11-Hydroxycorticoaldosterone
	11-«beta»,21-Dihydroxypregn-3,20-dione
	11-Â«betaÂ»,21-Dihydroxypregn-3,20-dione
	11Beta,21-dihydroxypregn-4-ene-3,20-dione
	11«beta»,21-Dihydroxyprogesterone
	11«beta»,21-dihydroxypregn-4-ene-3,20-dione
	11Â«betaÂ»,21-Dihydroxyprogesterone
	11Â«betaÂ»,21-dihydroxypregn-4-ene-3,20-dione
	17-Deoxycortisol
	4-Pregnen-11«beta»,21-diol-3,20-dione
	4-Pregnen-11Â«betaÂ»,21-diol-3,20-dione
	4-Pregnene-11«beta»,21-diol-3,20-dione
	4-Pregnene-11Â«betaÂ»,21-diol-3,20-dione
	Compound B
	Corticosteron
	Kendall's compound B
	NSC-9705
	Pregn-4-ene-3,20-dione, 11,21-dihydroxy-, (11«beta»)-
	Pregn-4-ene-3,20-dione, 11,21-dihydroxy-, (11Â«betaÂ»)-
	Pregn-4-ene-3,20-dione, 11«beta»,21-dihydroxy-
	Pregn-4-ene-3,20-dione, 11Â«betaÂ»,21-dihydroxy-
	Reichstein's B
	Reichstein's Substance H
Inchi:	InChI=1S/C21H30O4/c1-20-8-7-13(23)9-12(20)3-4-14-15-5-6-16(18(25)11-22)21(15,2)10
InchiKey:	OMFXVFTZEKFJBZ-UCINFPARSA-N
Formula:	C21H30O4
SMILES:	CC12CCC(=O)C=C1CCC1C2C(O)CC2(C)C(C(=O)CO)CCC12
Mol. weight [g/mol]:	346.46
CAS:	50-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-230.49	kJ/mol	Joback Method

hf	-755.34	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	104.93	kJ/mol	Joback Method
log10ws	-3.24		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-3.24		Estimated Solubility Method
log10ws	-3.24		Aqueous Solubility Prediction Method
logp	2.667		Crippen Method
mcvol	273.890	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	3341.10		NIST Webbook
rinpol	3341.10		NIST Webbook
tb	1024.85	K	Joback Method
tc	1260.06	K	Joback Method
tf	668.74	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.17	J/mol×K	1024.85	Joback Method
cpg	1100.46	J/mol×K	1064.05	Joback Method
cpg	1129.01	J/mol×K	1103.25	Joback Method
cpg	1159.12	J/mol×K	1142.45	Joback Method
cpg	1191.11	J/mol×K	1181.65	Joback Method
cpg	1225.31	J/mol×K	1220.85	Joback Method
cpg	1262.03	J/mol×K	1260.06	Joback Method
hfust	35.30	kJ/mol	458.50	NIST Webbook
hfust	33.32	kJ/mol	454.00	NIST Webbook

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50226&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

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