Aldosterone

Other names:	(+)-Aldosterone
	11«beta»,21-Dihydroxy-3,20-diketopregn-4-ene-18-al
	11«beta»,21-Dihydroxy-3,20-dioxo-pregn-4-en-18-al
	11«beta»,21-Dihydroxypregn-4-ene-3,18,20-trione
	11Â«betaÂ»,21-Dihydroxy-3,20-diketopregn-4-ene-18-al
	11Â«betaÂ»,21-Dihydroxy-3,20-dioxo-pregn-4-en-18-al
	11Â«betaÂ»,21-Dihydroxypregn-4-ene-3,18,20-trione
	18-Formyl-11«beta»,21-dihydroxy-4-pregnene-3,20-dione
	18-Formyl-11Â«betaÂ»,21-dihydroxy-4-pregnene-3,20-dione
	18-Oxocorticosterone
	Aldocorten
	Aldocortene
	Aldocortin
	D-Aldosterone
	Electrocortin
	Elektrocortin
	NSC 73856
	Pregn-4-en-18-al, 11,21-dihydroxy-3,20-dioxo-, (11«beta»)-
	Pregn-4-en-18-al, 11,21-dihydroxy-3,20-dioxo-, (11Â«betaÂ»)-
	Reichstein X
Inchi:	InChI=1S/C21H28O5/c1-20-7-6-13(24)8-12(20)2-3-14-15-4-5-16(18(26)10-22)21(15,11-2
InchiKey:	PQSUYGKTWSAVDQ-UHFFFAOYSA-N
Formula:	C21H28O5
SMILES:	CC12CCC(=O)C=C1CCC1C2C(O)CC2(C=O)C(C(=O)CO)CCC12
Mol. weight [g/mol]:	360.44
CAS:	52-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-330.01	kJ/mol	Joback Method
hf	-840.92	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	111.65	kJ/mol	Joback Method
log10ws	-3.85		Estimated Solubility Method
log10ws	-3.85		Aqueous Solubility Prediction Method

logp	1.846		Crippen Method
mcvol	275.460	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
tb	1073.51	K	Joback Method
tc	1316.26	K	Joback Method
tf	710.74	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.69	J/mol×K	1073.51	Joback Method
cpg	1125.82	J/mol×K	1113.97	Joback Method
cpg	1156.71	J/mol×K	1154.43	Joback Method
cpg	1189.71	J/mol×K	1194.89	Joback Method
cpg	1225.17	J/mol×K	1235.35	Joback Method
cpg	1263.43	J/mol×K	1275.80	Joback Method
cpg	1304.84	J/mol×K	1316.26	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52391&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume