Deoxycorticosterone

Other names:	11-Dehydroxycorticosterone
	11-Deoxycorticosterone
	11-Desoxycorticosterone
	21-Hydroxypregn-4-ene-3,20-dione
	21-Hydroxyprogesterone
	4-Pregnen-21-ol-3,20-dione
	Cortexone
	Corticosterone, 11-deoxy-
	DOC
	Deoxycortone
	Desoxycorticosterone
	Desoxycortone
	Kendall's Desoxy compound B
	NSC 11319
	Pregn-4-ene-3,20-dione, 21-hydroxy-
	Progesterone, 21-hydroxy-
	Reichstein's substance Q
Inchi:	InChI=1S/C21H30O3/c1-20-9-7-14(23)11-13(20)3-4-15-16-5-6-18(19(24)12-22)21(16,2)1
InchiKey:	ZESRJSPZRDMNHY-VQBCACJISA-N
Formula:	C21H30O3
SMILES:	CC12CCC(=O)C=C1CCC1C2CCC2(C)C(C(=O)CO)CCC12
Mol. weight [g/mol]:	330.46
CAS:	64-85-7

Physical Properties

Property code	Value	Unit	Source
chs	-12030.00 ± 4.00	kJ/mol	NIST Webbook
gf	-85.96	kJ/mol	Joback Method
hf	-582.77	kJ/mol	Joback Method
hfus	27.76	kJ/mol	Joback Method
hvap	88.56	kJ/mol	Joback Method
log10ws	-3.45		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-3.45		Estimated Solubility Method
log10ws	-3.59		Aqueous Solubility Prediction Method

logp	3.696		Crippen Method
mcvol	268.020	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	3106.60		NIST Webbook
tb	937.34	K	Joback Method
tc	1173.84	K	Joback Method
tf	414.82	K	Aqueous Solubility Prediction Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.08	J/mol×K	937.34	Joback Method
cpg	1015.67	J/mol×K	976.76	Joback Method
cpg	1041.90	J/mol×K	1016.17	Joback Method
cpg	1069.11	J/mol×K	1055.59	Joback Method
cpg	1097.62	J/mol×K	1095.00	Joback Method
cpg	1127.76	J/mol×K	1134.42	Joback Method
cpg	1159.85	J/mol×K	1173.84	Joback Method
hfust	27.98	kJ/mol	414.00	NIST Webbook

Sources

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

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=C64857&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion

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