Desoxycorticosterone Acetate

Other names:

11-Deoxycorticosterone 21-acetate
11-Deoxycorticosterone acetate
11-Desoxycorticosterone acetate
21-Acetoxy-3,20-diketopregn-4-ene
21-Acetoxypregn-4-en-3,20-dione
21-Acetoxypregn-4-ene-3,20-dione
21-Acetyloxypregn-4-ene-3,20-dione
21-Hydroxypregn-4-ene-3,20-dione 21-acetate
21-Hydroxypregn-4-ene-3,20-dione acetate
4-Pregnene-3,20-dione 21-acetate
4-Pregnene-3,20-dione-21-ol acetate
Arcort
Bio-Corten
Cortacet
Cortate
Cortenil
Cortesan
Cortexone acetate
Corticosterone, deoxy-, acetate
Cortifar
Cortigen
Cortinaq
Cortiron
Cortivis
Cortixyl
DCA
DOC acetate
DOCA
Decorten
Decortin
Decorton
Decosteron
Decosterone
Decostrate
Deoxycorticosterone 21-acetate
Deoxycorticosterone acetate
Deoxycortone acetate
Descornaq
Descorterone
Descotone

	Desocort
	Desoxycortone acetate
	Doc-Ac
	Doca acetate
	Docaquosum
	Dorcostrin
	Doxatone
	Doxo
	Doxycamon
	Krinocorts
	Mincortid
	Ocriten
	Ocritena
	Organon's doca acetate
	Percorten
	Percotol
	Pregn-4-ene-3,20-dione, 21-(acetyloxy)-
	Pregn-4-ene-3,20-dione, 21-hydroxy-, acetate
	Primocort
	Primocortan
	Sincortex
	Steraq
	Syncort
	Syncorta
	Syncortyl
	Unidocan
Inchi:	InChI=1S/C23H32O4/c1-14(24)27-13-21(26)20-7-6-18-17-5-4-15-12-16(25)8-10-22(15,2
InchiKey:	VPGRYOFKCNULNK-LCDLLCBDSA-N
Formula:	C23H32O4
SMILES:	CC(=O)OCC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	372.50
CAS:	56-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-166.22	kJ/mol	Joback Method
hf	-716.62	kJ/mol	Joback Method
hfus	31.64	kJ/mol	Joback Method
hvap	85.49	kJ/mol	Joback Method

log10ws	-4.63		Estimated Solubility Method
log10ws	-4.63		Aqueous Solubility Prediction Method
logp	4.267		Crippen Method
mcvol	297.770	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
tb	967.21	K	Joback Method
tc	1213.42	K	Joback Method
tf	646.04	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.57	J/mol×K	1172.39	Joback Method
cpg	1100.76	J/mol×K	967.21	Joback Method
cpg	1128.73	J/mol×K	1008.25	Joback Method
cpg	1157.35	J/mol×K	1049.28	Joback Method
cpg	1186.96	J/mol×K	1090.32	Joback Method
cpg	1217.92	J/mol×K	1131.35	Joback Method
cpg	1285.27	J/mol×K	1213.42	Joback Method
hfust	29.66	kJ/mol	430.00	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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56473&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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