Pregn-4-ene-3,20-dione, 19,21-dihydroxy-

Other names: 19-Hydroxydesoxycorticosterone
19,21-Dihydroxypregn-4-ene-3,20-dione
Inchi: InChI=1S/C21H30O4/c1-20-8-7-17-15(16(20)4-5-18(20)19(25)11-22)3-2-13-10-14(24)6-9
InchiKey: LFISWQXWWGJHBL-ZPMOIGASSA-N
Formula: C21H30O4
SMILES: CC12CCC3C(CCC4=CC(=O)CCC43CO)C1CCC2C(=O)CO
Mol. weight [g/mol]: 346.46
CAS: 2394-23-2

Physical Properties

Property code	Value	Unit	Source
gf	-222.78	kJ/mol	Joback Method
hf	-735.00	kJ/mol	Joback Method
hfus	31.85	kJ/mol	Joback Method
hvap	105.24	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.668		Crippen Method
mcvol	273.890	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
tb	1029.52	K	Joback Method
tc	1265.33	K	Joback Method
tf	672.98	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.74	J/mol×K	1029.52	Joback Method
cpg	1097.37	J/mol×K	1068.82	Joback Method
cpg	1126.40	J/mol×K	1108.12	Joback Method
cpg	1157.17	J/mol×K	1147.43	Joback Method
cpg	1190.01	J/mol×K	1186.73	Joback Method
cpg	1225.23	J/mol×K	1226.03	Joback Method
cpg	1263.17	J/mol×K	1265.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2394232&Units=SI
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

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