

Pregn-4-ene-3,20-dione, 14,21-dihydroxy-

Other names:	14«alpha»-Hydroxydeoxycorticosterone 14Alpha,21-dihydroxypregn-4-ene-3,20-dione
Inchi:	InChI=1S/C21H30O4/c1-19-8-5-14(23)11-13(19)3-4-16-15(19)6-9-20(2)17(18(24)12-22)
InchiKey:	XKCAPZYNIKDWOX-UHFFFAOYSA-N
Formula:	C21H30O4
SMILES:	CC12CCC(=O)C=C1CCC1C2CCC2(C)C(C(=O)CO)CCC12O
Mol. weight [g/mol]:	346.46
CAS:	595-71-1

Physical Properties

Property code	Value	Unit	Source
gf	-228.27	kJ/mol	Joback Method
hf	-719.76	kJ/mol	Joback Method
hfus	25.55	kJ/mol	Joback Method
hvap	104.09	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	2.811		Crippen Method
mvol	273.890	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
tb	1029.76	K	Joback Method
tc	1268.13	K	Joback Method
tf	696.88	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1081.15	J/molxK	1029.76	Joback Method
cpg	1115.41	J/molxK	1069.49	Joback Method
cpg	1152.45	J/molxK	1109.22	Joback Method
cpg	1192.71	J/molxK	1148.94	Joback Method
cpg	1236.66	J/molxK	1188.67	Joback Method
cpg	1284.74	J/molxK	1228.40	Joback Method
cpg	1337.41	J/molxK	1268.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C595711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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