Pregnane-3,20-dione, 11-hydroxy-, (5«alpha»,11«alpha»)-

Other names: 5«alpha»-Pregnane-3,20-dione, 11«alpha»-hydroxy-
11«alpha»-Hydroxyallopregnane-3,20-dione
11«alpha»-Hydroxy-5«alpha»-pregnane-3,20-dione
11Alpha-hydroxy-5alpha-pregnane-3,20-dione

Inchi: InChI=1S/C21H32O3/c1-12(22)16-6-7-17-15-5-4-13-10-14(23)8-9-20(13,2)19(15)18(24)1

InchiKey: XHCCPSKYYJBSAA-SZINYCQKSA-N

Formula: C21H32O3

SMILES: CC(=O)C1CCC2C3CCC4CC(=O)CCC4(C)C3C(O)CC12C

Mol. weight [g/mol]: 332.48

CAS: 565-96-8

Physical Properties

Property code	Value	Unit	Source
gf	-121.71	kJ/mol	Joback Method
hf	-669.76	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.774		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
tb	923.86	K	Joback Method
tc	1158.10	K	Joback Method
tf	590.40	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.31	J/mol×K	923.86	Joback Method
cpg	1053.52	J/mol×K	962.90	Joback Method
cpg	1080.03	J/mol×K	1001.94	Joback Method
cpg	1107.14	J/mol×K	1040.98	Joback Method
cpg	1135.16	J/mol×K	1080.02	Joback Method

cpg	1164.40	J/mol×K	1119.06	Joback Method
cpg	1195.17	J/mol×K	1158.10	Joback Method

Sources

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=C565968&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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