3«alpha»,21-dihydroxy-5«beta»-pregnane-11,20-d

Inchi: InChI=1S/C21H32O4/c1-20-8-7-14(22)9-12(20)3-5-15-16-6-4-13(10-18(24)25)21(16,2)11
InchiKey: JJLCXWVYRSJIRB-LOJQVEHYSA-N
Formula: C21H32O4
SMILES: CC12CC(=O)C3C(CCC4CC(O)CCC43C)C1CCC2CC(=O)O
Mol. weight [g/mol]: 348.48
CAS: 566-03-0

Physical Properties

Property code	Value	Unit	Source
gf	-258.53	kJ/mol	Joback Method
hf	-821.99	kJ/mol	Joback Method
hfus	33.16	kJ/mol	Joback Method
hvap	103.66	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.660		Crippen Method
mcvol	278.190	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2979.00		NIST Webbook
tb	1016.04	K	Joback Method
tc	1249.28	K	Joback Method
tf	651.22	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.45	J/mol×K	1016.04	Joback Method
cpg	1135.83	J/mol×K	1054.91	Joback Method
cpg	1164.23	J/mol×K	1093.79	Joback Method
cpg	1193.95	J/mol×K	1132.66	Joback Method
cpg	1225.29	J/mol×K	1171.53	Joback Method
cpg	1258.56	J/mol×K	1210.41	Joback Method
cpg	1294.07	J/mol×K	1249.28	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=C566030&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume