Androst-5-ene-16beta-propionic acid,3beta,17beta-dihydroxy-, delta-lactone

Inchi: InChI=1S/C22H32O3/c1-21-9-7-15(23)12-14(21)4-5-16-17(21)8-10-22(2)18(16)11-13-3-6

InchiKey: FQKKTVCAEAFHLR-UHFFFAOYSA-N

Formula: C22H32O3

SMILES: CC12CCC(O)CC1=CCC1C2CCC2(C)C1CC1CCC(=O)OC12

Mol. weight [g/mol]: 344.49

CAS: 96584-50-8

Physical Properties

Property code	Value	Unit	Source
gf	6.20	kJ/mol	Joback Method
hf	-576.53	kJ/mol	Joback Method
hfus	33.84	kJ/mol	Joback Method
hvap	88.32	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.242		Crippen Method
mcvol	275.550	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
tb	939.64	K	Joback Method
tc	1182.04	K	Joback Method
tf	610.25	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.34	J/mol×K	939.64	Joback Method
cpg	1087.29	J/mol×K	980.04	Joback Method
cpg	1115.88	J/mol×K	1020.44	Joback Method
cpg	1145.47	J/mol×K	1060.84	Joback Method
cpg	1176.46	J/mol×K	1101.24	Joback Method
cpg	1209.21	J/mol×K	1141.64	Joback Method
cpg	1244.09	J/mol×K	1182.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96584508&Units=SI

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