3Beta-acetoxy-17beta-hydroxy-5alpha-androstan-acid lactone

Inchi: InChI=1S/C23H34O4/c1-13(24)26-16-6-8-22(2)15(12-16)4-5-17-18(22)7-9-23(3)19(17)10

InchiKey: PAONJAURFWGCAT-UHFFFAOYSA-N

Formula: C23H34O4

SMILES: CC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C3CC3CC(=O)OC32)C1

Mol. weight [g/mol]: 374.51

CAS: 125567-32-0

Physical Properties

Property code	Value	Unit	Source
gf	-98.42	kJ/mol	Joback Method
hf	-750.23	kJ/mol	Joback Method
hfus	37.46	kJ/mol	Joback Method
hvap	81.59	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.502		Crippen Method
mcvol	295.510	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
tb	933.55	K	Joback Method
tc	1181.55	K	Joback Method
tf	618.86	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.12	J/mol×K	933.55	Joback Method
cpg	1162.79	J/mol×K	974.88	Joback Method
cpg	1192.81	J/mol×K	1016.22	Joback Method
cpg	1223.56	J/mol×K	1057.55	Joback Method
cpg	1255.42	J/mol×K	1098.88	Joback Method
cpg	1288.78	J/mol×K	1140.22	Joback Method
cpg	1324.02	J/mol×K	1181.55	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=C125567320&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