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

Inchi: InChI=1S/C24H34O4/c1-14(25)27-17-8-10-23(2)16(13-17)5-6-18-19(23)9-11-24(3)20(18
InchiKey: WXHAZWBPLJCITK-UHFFFAOYSA-N
Formula: C24H34O4
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C3CC3CCC(=O)OC32)C1
Mol. weight [g/mol]: 386.52
CAS: 96465-15-5

Physical Properties

Property code	Value	Unit	Source
gf	-74.06	kJ/mol	Joback Method
hf	-710.38	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	85.25	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.813		Crippen Method
mcvol	305.300	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
tb	969.51	K	Joback Method
tc	1222.02	K	Joback Method
tf	644.13	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.35	J/mol×K	969.51	Joback Method
cpg	1201.77	J/mol×K	1011.60	Joback Method
cpg	1232.84	J/mol×K	1053.68	Joback Method
cpg	1264.97	J/mol×K	1095.77	Joback Method
cpg	1298.55	J/mol×K	1137.85	Joback Method
cpg	1333.99	J/mol×K	1179.94	Joback Method
cpg	1371.70	J/mol×K	1222.02	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=C96465155&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