3Beta,17beta-diacetoxyandrost-5-ene

Inchi: InChI=1S/C23H34O4/c1-14(24)26-17-9-11-22(3)16(13-17)5-6-18-19-7-8-21(27-15(2)25)2
InchiKey: FKDRTPPOFBKQAT-UHFFFAOYSA-N
Formula: C23H34O4
SMILES: CC(=O)OC1C=C2CCC3C(CCC4(C)C(OC(C)=O)CCC34)C2(C)CC1
Mol. weight [g/mol]: 374.51
CAS: 4136-03-2

Physical Properties

Property code	Value	Unit	Source
gf	-156.34	kJ/mol	Joback Method
hf	-731.48	kJ/mol	Joback Method
hfus	34.39	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.813		Crippen Method
mcvol	302.070	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
tb	917.14	K	Joback Method
tc	1152.33	K	Joback Method
tf	595.81	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.99	J/mol×K	917.14	Joback Method
cpg	1118.88	J/mol×K	956.34	Joback Method
cpg	1145.99	J/mol×K	995.54	Joback Method
cpg	1173.62	J/mol×K	1034.74	Joback Method
cpg	1202.10	J/mol×K	1073.94	Joback Method
cpg	1231.74	J/mol×K	1113.14	Joback Method
cpg	1262.85	J/mol×K	1152.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4136032&Units=SI
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

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