A-norandrost-3(5)-en-2-one, 3,17-dihydroxy-, diacetate

Inchi: InChI=1S/C22H30O5/c1-12(23)26-19-8-7-15-14-5-6-17-20(27-13(2)24)18(25)11-22(17,4
InchiKey: HYYXLHSTZSNUIA-UHFFFAOYSA-N
Formula: C22H30O5
SMILES: CC(=O)OC1=C2CCC3C(CCC4(C)C(OC(C)=O)CCC34)C2(C)CC1=O
Mol. weight [g/mol]: 374.47
CAS: 1509-40-6

Physical Properties

Property code	Value	Unit	Source
gf	-277.17	kJ/mol	Joback Method
hf	-833.51	kJ/mol	Joback Method
hfus	31.95	kJ/mol	Joback Method
hvap	86.16	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.951		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
tb	967.46	K	Joback Method
tc	1210.38	K	Joback Method
tf	673.04	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.71	J/mol×K	967.46	Joback Method
cpg	1090.45	J/mol×K	1007.95	Joback Method
cpg	1117.81	J/mol×K	1048.43	Joback Method
cpg	1146.11	J/mol×K	1088.92	Joback Method
cpg	1175.65	J/mol×K	1129.41	Joback Method
cpg	1206.76	J/mol×K	1169.89	Joback Method
cpg	1239.74	J/mol×K	1210.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1509406&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