Androst-5-ene-3,17-diol, 3-acetate, (3«beta»,17«beta»)-

Other names: Androst-5-ene-3«beta»,17«beta»-diol, 3-acetate
Androstenediol 3-acetate
3«beta»-Acetoxy-5-androsten-17«beta»-ol
17-Hydroxyandrost-5-en-3-yl acetate, (3«beta»,17«beta»)-
3Beta-acetoxy-5-androsten-17beta-ol
17«beta»-hydroxyandrost-5-ene-3«beta»-yl acetate

Inchi: InChI=1S/C21H32O3/c1-13(22)24-15-8-10-20(2)14(12-15)4-5-16-17-6-7-19(23)21(17,3)1

InchiKey: OQHMNEGOKQMOFM-UHFFFAOYSA-N

Formula: C21H32O3

SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(O)CCC32)C1

Mol. weight [g/mol]: 332.48

CAS: 1639-43-6

Physical Properties

Property code	Value	Unit	Source
gf	-76.08	kJ/mol	Joback Method
hf	-597.63	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	86.41	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.242		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
tb	887.27	K	Joback Method
tc	1112.74	K	Joback Method
tf	561.93	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.61	J/mol×K	887.27	Joback Method
cpg	1007.12	J/mol×K	924.85	Joback Method
cpg	1031.85	J/mol×K	962.43	Joback Method

cpg	1057.07	J/mol×K	1000.01	Joback Method
cpg	1083.09	J/mol×K	1037.58	Joback Method
cpg	1110.21	J/mol×K	1075.16	Joback Method
cpg	1138.70	J/mol×K	1112.74	Joback Method

Sources

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=C1639436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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