

3Beta-acetoxy-11beta-hydroxy-5beta-androstan-1

Inchi:	InChI=1S/C21H32O4/c1-12(22)25-14-8-9-20(2)13(10-14)4-5-15-16-6-7-18(24)21(16,3)1
InchiKey:	CEFAOKKMPAXYIR-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CC(=O)OC1CCC2(C)C(CCC3C4CCC(=O)C4(C)CC(O)C32)C1
Mol. weight [g/mol]:	348.48
CAS:	3461-65-2

Physical Properties

Property code	Value	Unit	Source
gf	-226.71	kJ/mol	Joback Method
hf	-801.98	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	89.40	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.501		Crippen Method
mvol	278.190	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
tb	946.28	K	Joback Method
tc	1179.76	K	Joback Method
tf	612.63	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1061.00	J/molxK	946.28	Joback Method
cpg	1087.17	J/molxK	985.19	Joback Method
cpg	1113.66	J/molxK	1024.11	Joback Method
cpg	1140.75	J/molxK	1063.02	Joback Method
cpg	1168.72	J/molxK	1101.94	Joback Method
cpg	1197.86	J/molxK	1140.85	Joback Method
cpg	1228.45	J/molxK	1179.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3461652&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

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

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