

3Alpha,5alpha-cycloandrostandane, 6beta-acetamido-17beta-acetoxy-

Inchi:	InChI=1S/C23H35NO3/c1-13(25)24-19-11-16-17-5-6-20(27-14(2)26)21(17,3)9-8-18(16)2
InchiKey:	BLICXILAAZQDCC-UHFFFAOYSA-N
Formula:	C23H35NO3
SMILES:	CC(=O)NC1CC2C3CCC(OC(C)=O)C3(C)CCC2C2(C)CCC3CC312
Mol. weight [g/mol]:	373.53

Physical Properties

Property code	Value	Unit	Source
gf	101.57	kJ/mol	Joback Method
hf	-505.92	kJ/mol	Joback Method
hfus	36.68	kJ/mol	Joback Method
hvap	84.35	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.075		Crippen Method
mvol	299.620	ml/mol	McGowan Method
pc	1478.15	kPa	Joback Method
tb	930.25	K	Joback Method
tc	1166.07	K	Joback Method
tf	661.12	K	Joback Method
vc	1.147	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.90	J/mol×K	930.25	Joback Method
cpg	1164.05	J/mol×K	969.55	Joback Method
cpg	1198.08	J/mol×K	1008.86	Joback Method
cpg	1234.53	J/mol×K	1048.16	Joback Method
cpg	1273.90	J/mol×K	1087.47	Joback Method
cpg	1316.71	J/mol×K	1126.77	Joback Method
cpg	1363.48	J/mol×K	1166.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	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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