17Beta-acetylamino-16alpha-methyl-5-androsten-

Inchi: InChI=1S/C22H35NO2/c1-13-11-19-17-6-5-15-12-16(25)7-9-21(15,3)18(17)8-10-22(19,4

InchiKey: LGGHTNIMFTVTOB-UHFFFAOYSA-N

Formula: C22H35NO2

SMILES: CC(O)=NC1C(C)CC2C3CC=C4CC(O)CCC4(C)C3CCC21C

Mol. weight [g/mol]: 345.52

CAS: 95461-92-0

Physical Properties

Property code	Value	Unit	Source
hf	-473.61	kJ/mol	Joback Method
hvap	99.25	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.901		Crippen Method
mcvol	290.520	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
tb	997.93	K	Joback Method
tc	1228.42	K	Joback Method

Sources

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=C95461920&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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