Androst-6-ene-17beta-carboxylic acid, 3alpha-acetamido

Inchi: InChI=1S/C22H33NO3/c1-13(24)23-15-8-10-21(2)14(12-15)4-5-16-17-6-7-19(20(25)26)2

InchiKey: RDQLUVCEWHEPOU-UHFFFAOYSA-N

Formula: C22H33NO3

SMILES: CC(O)=NC1CCC2(C)C(=CCC3C2CCC2(C)C(C(=O)O)CCC32)C1

Mol. weight [g/mol]: 359.50

CAS: 5906-01-4

Physical Properties

Property code	Value	Unit	Source
hf	-565.85	kJ/mol	Joback Method
hvap	106.30	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.995		Crippen Method
mcvol	292.090	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
tb	1056.47	K	Joback Method
tc	1296.62	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5906014&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

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