17Beta-acetylamino-5-androsten-3beta-ol

Inchi: InChI=1S/C21H33NO2/c1-13(23)22-19-7-6-17-16-5-4-14-12-15(24)8-10-20(14,2)18(16)9
InchiKey: NOEHXIHMVNEQCJ-UHFFFAOYSA-N
Formula: C21H33NO2
SMILES: CC(O)=NC1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 331.49
CAS: 27508-62-9

Physical Properties

Property code	Value	Unit	Source
hf	-432.63	kJ/mol	Joback Method
hvap	97.33	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.655		Crippen Method
mcvol	276.430	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
tb	979.72	K	Joback Method
tc	1209.63	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27508629&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

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

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