5«alpha»-Androstan-3«beta»-ol-16-one, MO

Inchi: InChI=1S/C20H33NO2/c1-19-8-7-17-16(18(19)11-14(12-19)21-23-3)5-4-13-10-15(22)6-9
InchiKey: UBKSDCQZYWESSE-VPLGIVNPSA-N
Formula: C20H33NO2
SMILES: CON=C1CC2C3CCC4CC(O)CCC4(C)C3CCC2(C)C1
Mol. weight [g/mol]: 319.48

Physical Properties

Property code	Value	Unit	Source
hf	-469.69	kJ/mol	Joback Method
hvap	80.63	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.392		Crippen Method
mcvol	266.640	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2507.00		NIST Webbook
tb	885.54	K	Joback Method
tc	1114.90	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R523292&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature