5«beta»-Androstan-3«alpha»,11«beta»-diol-17-on
(Androsterone), MO

Inchi: InChI=1S/C20H33NO3/c1-19-9-8-13(22)10-12(19)4-5-14-15-6-7-17(21-24-3)20(15,2)11-1

InchiKey: UZMRRBJCQIXXCE-SQSLJORLSA-N

Formula: C20H33NO3

SMILES: CON=C1CCC2C3CCC4CC(O)CCC4(C)C3C(O)CC12C

Mol. weight [g/mol]: 335.48

Physical Properties

Property code	Value	Unit	Source
hf	-642.26	kJ/mol	Joback Method
hvap	97.00	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.363		Crippen Method
mcvol	272.510	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2622.00		NIST Webbook
tb	973.05	K	Joback Method
tc	1199.28	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R523089&Units=SI

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

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