5«alpha»-Androstan-17-one, MO

Inchi: InChI=1S/C20H31NO2/c1-19-10-8-14(22)12-13(19)4-5-15-16-6-7-18(21-23-3)20(16,2)11
InchiKey: RDKMQXKUDOHVAO-FCRDDDDSSA-N
Formula: C20H31NO2
SMILES: CON=C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 317.47

Physical Properties

Property code	Value	Unit	Source
hf	-434.82	kJ/mol	Joback Method
hvap	68.51	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.601		Crippen Method
mcvol	262.340	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	2243.00		NIST Webbook
tb	865.85	K	Joback Method
tc	1119.33	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=R523252&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature