Androstenedione, MO-TMS

Other names: Androst-4-ene-3,17-dione, 3,17-diMO
Inchi: InChI=1S/C21H32N2O2/c1-20-11-9-15(22-24-3)13-14(20)5-6-16-17-7-8-19(23-25-4)21(1
InchiKey: ZZDSWSPDFBFXIQ-ORPNCOOFSA-N
Formula: C21H32N2O2
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
hf	-342.30	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.954		Crippen Method
mcvol	282.110	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tb	931.30	K	Joback Method
tc	1179.68	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3091369&Units=SI

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