Methyl 17A-hydroxy-3-oxoandrost-4-ene-17B-carboxylate 3-MO

Inchi: InChI=1S/C22H33NO4/c1-20-10-7-15(23-27-4)13-14(20)5-6-16-17(20)8-11-21(2)18(16)9

InchiKey: VZCXPYYTJKLYDM-UFTDUSJJSA-N

Formula: C22H33NO4

SMILES: CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O)C(=O)OC)C2(C)CC1

Mol. weight [g/mol]: 375.50

Physical Properties

Property code	Value	Unit	Source
hf	-673.88	kJ/mol	Joback Method
hvap	94.35	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.856		Crippen Method
mcvol	297.960	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	2840.00		NIST Webbook
tb	1016.64	K	Joback Method
tc	1256.81	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=R93145&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