3-Oxoandrost-4-ene-17B-carboxaldehyde, 3,20-diMO

Inchi: InChI=1S/C22H34N2O2/c1-21-11-9-17(24-26-4)13-15(21)5-7-18-19-8-6-16(14-23-25-3)2

InchiKey: SWIRRSJJIZIZFT-LUMBAORHSA-N

Formula: C22H34N2O2

SMILES: CON=CC1CCC2C3CCC4=CC(=NOC)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 358.52

Physical Properties

Property code	Value	Unit	Source
hf	-342.09	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	5.200		Crippen Method
mcvol	296.200	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	947.03	K	Joback Method
tc	1194.38	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R93056&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