5-«beta»-Pregnan-3,11-dione, MO

Inchi: InChI=1S/C23H38N2O2/c1-6-15-8-10-19-18-9-7-16-13-17(24-26-4)11-12-22(16,2)21(18)
InchiKey: ACPIXOASZHBQJM-QYUPGOEQSA-N
Formula: C23H38N2O2
SMILES: CCC1CCC2C3CCC4CC(=NOC)CCC4(C)C3C(=NOC)CC12C
Mol. weight [g/mol]: 374.56

Physical Properties

Property code	Value	Unit	Source
hf	-470.57	kJ/mol	Joback Method
hvap	77.18	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.670		Crippen Method
mcvol	314.590	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	2536.00		NIST Webbook
rinpol	2536.00		NIST Webbook
tb	963.58	K	Joback Method
tc	1204.81	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=R486925&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