17«alpha»-Hydroxyprogesterone, bis(O-methyloxime)

Other names: 17«alpha»-Hydroxyprogesterone, 3,20-bis-MO
Inchi: InChI=1S/C23H36N2O3/c1-15(24-27-4)23(26)13-10-20-18-7-6-16-14-17(25-28-5)8-11-21
InchiKey: FTLBXAHUQAJCNR-UHFFFAOYSA-N
Formula: C23H36N2O3
SMILES: CON=C1C=C2CCC3C(CCC4(C)C3CCC4(O)C(C)=NOC)C2(C)CC1
Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
hf	-509.51	kJ/mol	Joback Method
hvap	93.22	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.705		Crippen Method
mcvol	316.160	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
tb	1062.21	K	Joback Method
tc	1309.61	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U394526&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature