Androst-5-en-17-one-3beta- nitrite

Inchi: InChI=1S/C19H27NO3/c1-18-9-7-13(23-20-22)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10
InchiKey: HXNFSAGZLTWCLH-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CC12CCC3C(CC=C4CC(ON=O)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 317.42
CAS: 99099-00-0

Physical Properties

Property code	Value	Unit	Source
hf	-577.09	kJ/mol	Joback Method
hvap	72.19	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.585		Crippen Method
mcvol	249.820	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
tb	831.35	K	Joback Method
tc	1075.66	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=C99099000&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature