4-Androsten-3,17-dione dimethoxime

Other names: Androst-4-ene-3,17-dione, 3,17-diMO
Inchi: InChI=1S/C21H32N2O2/c1-20-11-9-15(22-24-3)13-14(20)5-6-16-17-7-8-19(23-25-4)21(1
InchiKey: ZZDSWSPDFBFXIQ-ORPNCOOFSA-N
Formula: C21H32N2O2
SMILES: CON=C1C=C2CCC3C(CCC4(C)C(=NOC)CCC34)C2(C)CC1
Mol. weight [g/mol]: 344.49
CAS: 3091-36-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Cheméo Relay (1.0)
logp	4.954		Crippen Method
mcvol	282.110	ml/mol	McGowan Method
rinpol	2690.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tf	377.65	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3091369&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point