

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-OEUJLIAZSA-N
Formula:	C21H32N2O2
SMILES:	CON=C1C=C2CC[C@@H]3[C@H](CC[C@]4(C)C(=NOC)CC[C@@H]34)[C@@]2(C)CC
Mol. weight [g/mol]:	344.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Cheméo Relay (1.0)
logp	4.954		Crippen Method
mcvol	282.110	ml/mol	McGowan Method
tf	378.80	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3091369&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

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