

Androst-4-en-3-one, 17-hydroxy-, O-methyloxime, (17«beta»)-

Other names:	4-Androsten-17«beta»-ol-3-one (testosterone), MO
Inchi:	InChI=1S/C20H31NO2/c1-19-10-8-14(21-23-3)12-13(19)4-5-15-16-6-7-18(22)20(16,2)11
InchiKey:	OCGJMJC BENBXGY-BZIXAJQCSA-N
Formula:	C20H31NO2
SMILES:	CON=C1C=C2CCC3C(CCC4(C)C(O)CCC34)C2(C)CC1
Mol. weight [g/mol]:	317.47
CAS:	3091-89-2

Physical Properties

Property code	Value	Unit	Source
hf	-403.04	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.312		Crippen Method
mcvol	262.340	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	894.35	K	Joback Method
tc	1125.87	K	Joback Method

Sources

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=C3091892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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