

Testosterone, 3,17«beta»-bisAc

Inchi:	InChI=1S/C23H32O4/c1-14(24)26-17-9-11-22(3)16(13-17)5-6-18-19-7-8-21(27-15(2)25)2
InchiKey:	BHBZEDXYAXMCOT-IYEFYMBESA-N
Formula:	C23H32O4
SMILES:	CC(=O)OC1=CCC2(C)C(=C1)CCC1C2CCC2(C)C(OC(C)=O)CCC12
Mol. weight [g/mol]:	372.50

Physical Properties

Property code	Value	Unit	Source
gf	-128.30	kJ/mol	Joback Method
hf	-664.83	kJ/mol	Joback Method
hfus	34.15	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.938		Crippen Method
mvol	297.770	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	2726.00		NIST Webbook
rinpol	2726.00		NIST Webbook
tb	925.95	K	Joback Method
tc	1163.28	K	Joback Method
tf	613.33	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.60	J/mol×K	925.95	Joback Method
cpg	1084.86	J/mol×K	965.50	Joback Method
cpg	1111.55	J/mol×K	1005.06	Joback Method
cpg	1139.00	J/mol×K	1044.61	Joback Method
cpg	1167.55	J/mol×K	1084.17	Joback Method
cpg	1197.51	J/mol×K	1123.72	Joback Method
cpg	1229.22	J/mol×K	1163.28	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=R135607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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