

Testosterone, HFB

Inchi: InChI=1S/C23H27F7O3/c1-19-9-7-13(31)11-12(19)3-4-14-15-5-6-17(20(15,2)10-8-16(14)
InchiKey: ZRANHFFRDGWPRP-XVBHISAFSA-N
Formula: C23H27F7O3
SMILES: CC12CCC(=O)C=C1CCC1C2CCC2(C)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CCC12
Mol. weight [g/mol]: 484.45

Physical Properties

Property code	Value	Unit	Source
gf	-1392.45	kJ/mol	Joback Method
hf	-2003.06	kJ/mol	Joback Method
hfus	29.36	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.263		Crippen Method
mvol	308.590	ml/mol	McGowan Method
pc	1178.47	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	898.54	K	Joback Method
tc	1117.72	K	Joback Method
tf	607.50	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1122.35	J/molxK	898.54	Joback Method
cpg	1145.66	J/molxK	935.07	Joback Method
cpg	1169.24	J/molxK	971.60	Joback Method
cpg	1193.40	J/molxK	1008.13	Joback Method
cpg	1218.47	J/molxK	1044.66	Joback Method
cpg	1244.77	J/molxK	1081.19	Joback Method
cpg	1272.64	J/molxK	1117.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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