

Testosterone, 3,17«beta»-bis-chlorodifluoroacetate

Inchi: InChI=1S/C23H26Cl2F4O4/c1-20-9-7-13(32-18(30)22(24,26)27)11-12(20)3-4-14-15-5-6-
InchiKey: LPASLVRGRICJCI-FVLSIOMWSA-N
Formula: C23H26Cl2F4O4
SMILES: CC12CC=C(OC(=O)C(F)(F)Cl)C=C1CCC1C2CCC2(C)C(OC(=O)C(F)(F)Cl)CCC12
Mol. weight [g/mol]: 513.35

Physical Properties

Property code	Value	Unit	Source
gf	-925.72	kJ/mol	Joback Method
hf	-1498.25	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	87.51	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	6.561		Crippen Method
mcvol	329.330	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2728.00		NIST Webbook
tb	991.43	K	Joback Method
tc	1226.98	K	Joback Method
tf	680.37	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.35	J/mol×K	991.43	Joback Method
cpg	1176.02	J/mol×K	1030.69	Joback Method
cpg	1203.01	J/mol×K	1069.95	Joback Method
cpg	1231.73	J/mol×K	1109.20	Joback Method
cpg	1262.54	J/mol×K	1148.46	Joback Method
cpg	1295.84	J/mol×K	1187.72	Joback Method
cpg	1332.02	J/mol×K	1226.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R135612&Units=SI

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

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