Testosterone, 3-HFB, 17«beta»-monochloacetate

Inchi: InChI=1S/C25H28ClF7O4/c1-21-9-7-14(36-20(35)23(27,28)24(29,30)25(31,32)33)11-13(

InchiKey: WYBQRJXFEKTTGH-FSFORYKRSA-N

Formula: C25H28ClF7O4

SMILES: CC12CC=C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C=C1CCC1C2CCC2(C)C(OC(=O)CCl)CCC

Mol. weight [g/mol]: 560.93

Physical Properties

Property code	Value	Unit	Source
gf	-1478.54	kJ/mol	Joback Method
hf	-2120.87	kJ/mol	Joback Method
hfus	42.85	kJ/mol	Joback Method
hvap	83.83	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	6.970		Crippen Method
mcvol	350.580	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2795.00		NIST Webbook
tb	994.34	K	Joback Method
tc	1220.42	K	Joback Method
tf	677.18	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.60	J/mol×K	994.34	Joback Method
cpg	1295.66	J/mol×K	1032.02	Joback Method
cpg	1322.99	J/mol×K	1069.70	Joback Method
cpg	1351.96	J/mol×K	1107.38	Joback Method
cpg	1382.94	J/mol×K	1145.06	Joback Method
cpg	1416.32	J/mol×K	1182.74	Joback Method
cpg	1452.47	J/mol×K	1220.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R135701&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