Testosterone, 3,17«beta»-bispentafluoropropionate

Inchi: InChI=1S/C25H26F10O4/c1-20-9-7-13(38-18(36)22(26,27)24(30,31)32)11-12(20)3-4-14-

InchiKey: GTHFNBCICDBBFH-RZCFPABXSA-N

Formula: C25H26F10O4

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

Mol. weight [g/mol]: 580.46

Physical Properties

Property code	Value	Unit	Source
gf	-2048.20	kJ/mol	Joback Method
hf	-2702.21	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	75.70	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	7.293		Crippen Method
mcvol	343.650	ml/mol	McGowan Method
pc	983.31	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	951.49	K	Joback Method
tc	1166.61	K	Joback Method
tf	651.45	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.90	J/mol×K	951.49	Joback Method
cpg	1279.39	J/mol×K	987.34	Joback Method
cpg	1303.71	J/mol×K	1023.20	Joback Method
cpg	1329.22	J/mol×K	1059.05	Joback Method
cpg	1356.25	J/mol×K	1094.90	Joback Method
cpg	1385.16	J/mol×K	1130.76	Joback Method
cpg	1416.28	J/mol×K	1166.61	Joback Method

Sources

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=R135632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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