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

Inchi: InChI=1S/C26H26F12O4/c1-20-9-7-13(41-19(40)23(29,30)25(33,34)35)11-12(20)3-4-14-

InchiKey: USLXJCDJCHXXGL-FVLSIOMWSA-N

Formula: C26H26F12O4

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

Mol. weight [g/mol]: 630.46

Physical Properties

Property code	Value	Unit	Source
gf	-2426.56	kJ/mol	Joback Method
hf	-3123.82	kJ/mol	Joback Method
hfus	41.81	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	7.929		Crippen Method
mcvol	361.280	ml/mol	McGowan Method
pc	887.88	kPa	Joback Method
rinpol	2402.00		NIST Webbook
tb	969.68	K	Joback Method
tc	1187.21	K	Joback Method
tf	666.32	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1334.61	J/mol×K	969.68	Joback Method
cpg	1359.14	J/mol×K	1005.93	Joback Method
cpg	1384.79	J/mol×K	1042.19	Joback Method
cpg	1411.93	J/mol×K	1078.44	Joback Method
cpg	1440.95	J/mol×K	1114.70	Joback Method
cpg	1472.24	J/mol×K	1150.95	Joback Method
cpg	1506.17	J/mol×K	1187.21	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=R135761&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