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

Inchi: InChI=1S/C31H26F22O4/c1-20-9-7-13(56-18(54)23(34,35)25(38,39)30(48,49)50)11-12(2

InchiKey: RFVFRSOMSJOGTE-FVLSIOMWSA-N

Formula: C31H26F22O4

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

Mol. weight [g/mol]: 880.50

Physical Properties

Property code	Value	Unit	Source
gf	-4318.36	kJ/mol	Joback Method
hf	-5231.87	kJ/mol	Joback Method
hfus	48.49	kJ/mol	Joback Method
hvap	71.48	kJ/mol	Joback Method
log10ws	-13.05		Crippen Method
logp	11.105		Crippen Method
mcvol	449.430	ml/mol	McGowan Method
pc	569.33	kPa	Joback Method
rinpol	2625.00		NIST Webbook
rinpol	2625.00		NIST Webbook
tb	1060.63	K	Joback Method
tc	1329.83	K	Joback Method
tf	740.67	K	Joback Method
vc	1.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1738.42	J/mol×K	1060.63	Joback Method
cpg	1777.40	J/mol×K	1105.50	Joback Method
cpg	1820.83	J/mol×K	1150.36	Joback Method
cpg	1869.69	J/mol×K	1195.23	Joback Method
cpg	1924.96	J/mol×K	1240.10	Joback Method
cpg	1987.63	J/mol×K	1284.96	Joback Method
cpg	2058.69	J/mol×K	1329.83	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=R135716&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