Androst-5,9(11)-diene-3-«beta»,17-«beta»-diol, TFA

Inchi: InChI=1S/C23H26F6O4/c1-20-9-7-13(32-18(30)22(24,25)26)11-12(20)3-4-14-15-5-6-17(

InchiKey: OAPUIKPISZUEDE-WKCVYIDDSA-N

Formula: C23H26F6O4

SMILES: CC12CCC(OC(=O)C(F)(F)F)CC1=CCC1C2=CCC2(C)C(OC(=O)C(F)(F)F)CCC12

Mol. weight [g/mol]: 480.44

Physical Properties

Property code	Value	Unit	Source
gf	-1291.48	kJ/mol	Joback Method
hf	-1858.99	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	77.11	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.817		Crippen Method
mcvol	308.390	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
tb	915.11	K	Joback Method
tc	1132.21	K	Joback Method
tf	621.71	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.84	J/mol×K	915.11	Joback Method
cpg	1122.38	J/mol×K	951.29	Joback Method
cpg	1145.35	J/mol×K	987.48	Joback Method
cpg	1169.06	J/mol×K	1023.66	Joback Method
cpg	1193.81	J/mol×K	1059.84	Joback Method
cpg	1219.89	J/mol×K	1096.03	Joback Method
cpg	1247.61	J/mol×K	1132.21	Joback Method

Sources

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=R385372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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