5-Androsten-3-«beta»,17-«beta»-diol, TFA

Inchi: InChI=1S/C23H28F6O4/c1-20-9-7-13(32-18(30)22(24,25)26)11-12(20)3-4-14-15-5-6-17(
InchiKey: OAFQCHNBNINGJD-NZOVMWNSSA-N
Formula: C23H28F6O4
SMILES: CC12CCC(OC(=O)C(F)(F)F)CC1=CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12
Mol. weight [g/mol]: 482.46

Physical Properties

Property code	Value	Unit	Source
gf	-1319.52	kJ/mol	Joback Method
hf	-1925.64	kJ/mol	Joback Method
hfus	38.04	kJ/mol	Joback Method
hvap	75.85	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.897		Crippen Method
mcvol	312.690	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	906.30	K	Joback Method
tc	1121.39	K	Joback Method
tf	604.19	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.31	J/mol×K	906.30	Joback Method
cpg	1156.47	J/mol×K	942.15	Joback Method
cpg	1179.86	J/mol×K	978.00	Joback Method
cpg	1203.78	J/mol×K	1013.84	Joback Method
cpg	1228.51	J/mol×K	1049.69	Joback Method
cpg	1254.35	J/mol×K	1085.54	Joback Method
cpg	1281.59	J/mol×K	1121.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R385307&Units=SI
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

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