5-«alpha»-Androstan-3-«beta»,16-«alpha»-diol, TFA

InChI: InChI=1S/C23H30F6O4/c1-20-7-6-16-15(17(20)10-14(11-20)33-19(31)23(27,28)29)4-3-1
InchiKey: QRLGIKUCSMWAQY-SPZQWNDZSA-N
Formula: C23H30F6O4
SMILES: CC12CCC3C(CCC4CC(OC(=O)C(F)(F)F)CCC43C)C1CC(OC(=O)C(F)(F)F)C2
Mol. weight [g/mol]: 484.47

Physical Properties

Property code	Value	Unit	Source
gf	-1347.56	kJ/mol	Joback Method
hf	-1992.29	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	74.58	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.977		Crippen Method
mcvol	316.990	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2344.00		NIST Webbook
tb	897.49	K	Joback Method
tc	1110.56	K	Joback Method
tf	586.67	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.32	J/mol×K	897.49	Joback Method
cpg	1190.15	J/mol×K	933.00	Joback Method
cpg	1214.03	J/mol×K	968.51	Joback Method
cpg	1238.23	J/mol×K	1004.03	Joback Method
cpg	1263.04	J/mol×K	1039.54	Joback Method
cpg	1288.73	J/mol×K	1075.05	Joback Method
cpg	1315.58	J/mol×K	1110.56	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=R384804&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