5-«alpha»-Androst-1-ene-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: XEHYQXGMKFCQLK-KPNBZLMOSA-N

Formula: C23H28F6O4

SMILES: CC12C=CC(OC(=O)C(F)(F)F)CC1CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12

Mol. weight [g/mol]: 482.46

Physical Properties

Property code	Value	Unit	Source
gf	-1317.60	kJ/mol	Joback Method
hf	-1934.51	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	74.88	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.753		Crippen Method
mcvol	312.690	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	2364.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	896.65	K	Joback Method
tc	1110.46	K	Joback Method
tf	587.43	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.57	J/mol×K	896.65	Joback Method
cpg	1159.70	J/mol×K	932.29	Joback Method
cpg	1182.93	J/mol×K	967.92	Joback Method
cpg	1206.54	J/mol×K	1003.56	Joback Method
cpg	1230.82	J/mol×K	1039.19	Joback Method
cpg	1256.06	J/mol×K	1074.83	Joback Method
cpg	1282.53	J/mol×K	1110.46	Joback Method

Sources

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=R384691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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