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

Inchi: InChI=1S/C27H26F14O4/c1-20-9-7-13(44-18(42)22(28,29)24(32,33)26(36,37)38)11-12(2

InchiKey: UCBYJFZGAXTFFC-WKCVYIDDSA-N

Formula: C27H26F14O4

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

Mol. weight [g/mol]: 680.47

Physical Properties

Property code	Value	Unit	Source
gf	-2804.92	kJ/mol	Joback Method
hf	-3545.43	kJ/mol	Joback Method
hfus	43.15	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	8.359		Crippen Method
mcvol	378.910	ml/mol	McGowan Method
pc	805.70	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	987.87	K	Joback Method
tc	1210.22	K	Joback Method
tf	681.19	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.87	J/mol×K	987.87	Joback Method
cpg	1439.92	J/mol×K	1024.93	Joback Method
cpg	1467.43	J/mol×K	1061.99	Joback Method
cpg	1496.84	J/mol×K	1099.05	Joback Method
cpg	1528.60	J/mol×K	1136.10	Joback Method
cpg	1563.13	J/mol×K	1173.16	Joback Method
cpg	1600.88	J/mol×K	1210.22	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=R385367&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