5-Androsten-3-«alpha»,17-«beta»-diol, HFB

Inchi: InChI=1S/C27H28F14O4/c1-20-9-7-13(44-18(42)22(28,29)24(32,33)26(36,37)38)11-12(2
InchiKey: LOQSLZRGIFRAMO-SYJHMIIESA-N
Formula: C27H28F14O4
SMILES: CC12CCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)CC1=CCC1C2CCC2(C)C(OC(=O)C(F)(F)C(F
Mol. weight [g/mol]: 682.49

Physical Properties

Property code	Value	Unit	Source
gf	-2832.96	kJ/mol	Joback Method
hf	-3612.08	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	73.03	kJ/mol	Joback Method
log10ws	-9.88		Crippen Method
logp	8.439		Crippen Method
mcvol	383.210	ml/mol	McGowan Method
pc	781.56	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2352.00		NIST Webbook
tb	979.06	K	Joback Method
tc	1199.41	K	Joback Method
tf	663.67	K	Joback Method
vc	1.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1448.45	J/mol×K	979.06	Joback Method
cpg	1474.64	J/mol×K	1015.78	Joback Method
cpg	1502.03	J/mol×K	1052.51	Joback Method
cpg	1531.05	J/mol×K	1089.23	Joback Method
cpg	1562.13	J/mol×K	1125.96	Joback Method
cpg	1595.68	J/mol×K	1162.68	Joback Method
cpg	1632.13	J/mol×K	1199.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R385243&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

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