6«beta»-Hydroxy-3«alpha», 5«alpha»-cycloandrostan-17-one, TFA

Inchi: InChI=1S/C21H27F3O3/c1-18-7-6-14-12(13(18)3-4-16(18)25)5-8-20(27-17(26)21(22,23)

InchiKey: BISGMCOZQUQHBY-NJGCBKJZSA-N

Formula: C21H27F3O3

SMILES: CC12CCC3C(CCC4(OC(=O)C(F)(F)F)C5CC5CC34C)C1CCC2=O

Mol. weight [g/mol]: 384.43

Physical Properties

Property code	Value	Unit	Source
gf	-572.21	kJ/mol	Joback Method
hf	-1119.97	kJ/mol	Joback Method
hfus	25.06	kJ/mol	Joback Method
hvap	67.52	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.682		Crippen Method
mcvol	266.770	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	2404.00		NIST Webbook
tb	847.52	K	Joback Method
tc	1079.23	K	Joback Method
tf	612.64	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.96	J/mol×K	847.52	Joback Method
cpg	992.09	J/mol×K	886.14	Joback Method
cpg	1019.13	J/mol×K	924.76	Joback Method
cpg	1047.57	J/mol×K	963.38	Joback Method
cpg	1077.90	J/mol×K	1001.99	Joback Method
cpg	1110.59	J/mol×K	1040.61	Joback Method
cpg	1146.12	J/mol×K	1079.23	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=R305232&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

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