17-epi-Bolasterone

Inchi: InChI=1S/C21H32O2/c1-13-11-14-12-15(22)5-8-19(14,2)16-6-9-20(3)17(18(13)16)7-10-2
InchiKey: IVFYLRMMHVYGJH-YGZWZPPASA-N
Formula: C21H32O2
SMILES: CC1CC2=CC(=O)CCC2(C)C2CCC3(C)C(CCC3(C)O)C12
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	29.76	kJ/mol	Joback Method
hf	-475.29	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.515		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	2722.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	879.04	K	Joback Method
tc	1115.52	K	Joback Method
tf	581.89	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.45	J/mol×K	879.04	Joback Method
cpg	993.76	J/mol×K	918.45	Joback Method
cpg	1023.08	J/mol×K	957.87	Joback Method
cpg	1053.82	J/mol×K	997.28	Joback Method
cpg	1086.44	J/mol×K	1036.69	Joback Method
cpg	1121.35	J/mol×K	1076.11	Joback Method
cpg	1158.99	J/mol×K	1115.52	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=R257688&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