7-«alpha»,17-«beta»-Dimethyl-5-«beta»-Androstan

Inchi: InChI=1S/C21H36O2/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: ZWQUPIDNCOVROC-SBXJRRCCSA-N
Formula: C21H36O2
SMILES: CC1CC2CC(O)CCC2(C)C2CCC3(C)C(CCC3(C)O)C12
Mol. weight [g/mol]: 320.51

Physical Properties

Property code	Value	Unit	Source
gf	-20.22	kJ/mol	Joback Method
hf	-576.81	kJ/mol	Joback Method
hfus	26.82	kJ/mol	Joback Method
hvap	91.21	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.387		Crippen Method
mcvol	275.050	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2614.00		NIST Webbook
rinpol	2614.00		NIST Webbook
tb	889.92	K	Joback Method
tc	1106.54	K	Joback Method
tf	552.73	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.16	J/mol×K	889.92	Joback Method
cpg	1063.65	J/mol×K	926.02	Joback Method
cpg	1092.05	J/mol×K	962.13	Joback Method
cpg	1121.72	J/mol×K	998.23	Joback Method
cpg	1153.00	J/mol×K	1034.33	Joback Method
cpg	1186.26	J/mol×K	1070.43	Joback Method
cpg	1221.85	J/mol×K	1106.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R258136&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