Androstan-3-one, (5alpha), 11beta,17beta-dihydroxy-17alpha-methyl-

Inchi: InChI=1S/C20H32O3/c1-18-8-6-13(21)10-12(18)4-5-14-15-7-9-20(3,23)19(15,2)11-16(22

InchiKey: RNPQQCQDRWIESD-UHFFFAOYSA-N

Formula: C20H32O3

SMILES: CC12CCC(=O)CC1CCC1C2C(O)CC2(C)C1CCC2(C)O

Mol. weight [g/mol]: 320.47

CAS: 5454-55-7

Physical Properties

Property code	Value	Unit	Source
gf	-143.52	kJ/mol	Joback Method
hf	-673.53	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	93.54	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.320		Crippen Method
mcvol	262.530	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
tb	939.53	K	Joback Method
tc	1167.54	K	Joback Method
tf	613.92	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.35	J/mol×K	939.53	Joback Method
cpg	1046.31	J/mol×K	977.53	Joback Method
cpg	1076.72	J/mol×K	1015.53	Joback Method
cpg	1108.96	J/mol×K	1053.54	Joback Method
cpg	1143.42	J/mol×K	1091.54	Joback Method
cpg	1180.49	J/mol×K	1129.54	Joback Method
cpg	1220.53	J/mol×K	1167.54	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=C5454557&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume