6Beta-hydroxyandrost-4-ene-3,17-dione

Inchi: InChI=1S/C19H26O3/c1-18-7-5-11(20)9-15(18)16(21)10-12-13-3-4-17(22)19(13,2)8-6-14
InchiKey: WVAMBAWFDOYFOD-RITAXZTOSA-N
Formula: C19H26O3
SMILES: CC12CCC3C(CC(O)C4=CC(=O)CCC43C)C1CCC2=O
Mol. weight [g/mol]: 302.41
CAS: 63-00-3

Physical Properties

Property code	Value	Unit	Source
gf	-96.47	kJ/mol	Joback Method
hf	-566.61	kJ/mol	Joback Method
hfus	20.49	kJ/mol	Joback Method
hvap	81.61	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.058		Crippen Method
mcvol	239.840	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	905.53	K	Joback Method
tc	1151.14	K	Joback Method
tf	607.91	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.55	J/mol×K	905.53	Joback Method
cpg	905.20	J/mol×K	946.47	Joback Method
cpg	930.17	J/mol×K	987.40	Joback Method
cpg	955.78	J/mol×K	1028.34	Joback Method
cpg	982.35	J/mol×K	1069.27	Joback Method
cpg	1010.19	J/mol×K	1110.21	Joback Method
cpg	1039.62	J/mol×K	1151.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63003&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume