5«beta»,17«alpha»-Dihydroepitestosterone methanoate

Inchi: InChI=1S/C20H30O3/c1-19-9-7-14(22)11-13(19)3-4-15-16-5-6-18(23-12-21)20(16,2)10-8

InchiKey: ZQSXNBHXKJQHBH-HIBXAUDXSA-N

Formula: C20H30O3

SMILES: CC12CCC(=O)CC1CCC1C2CCC2(C)C(OC=O)CCC12

Mol. weight [g/mol]: 318.45

Physical Properties

Property code	Value	Unit	Source
gf	-61.20	kJ/mol	Joback Method
hf	-581.77	kJ/mol	Joback Method
hfus	23.20	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.140		Crippen Method
mcvol	258.230	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	2513.82		NIST Webbook
rinpol	2525.92		NIST Webbook
tb	830.68	K	Joback Method
tc	1076.08	K	Joback Method
tf	536.85	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.89	J/mol×K	830.68	Joback Method
cpg	939.50	J/mol×K	871.58	Joback Method
cpg	965.71	J/mol×K	912.48	Joback Method
cpg	991.87	J/mol×K	953.38	Joback Method
cpg	1018.30	J/mol×K	994.28	Joback Method
cpg	1045.36	J/mol×K	1035.18	Joback Method
cpg	1073.36	J/mol×K	1076.08	Joback Method

Sources

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=R190382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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