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

Inchi: InChI=1S/C23H36O3/c1-4-5-21(25)26-20-9-8-18-17-7-6-15-14-16(24)10-12-22(15,2)19(1

InchiKey: RRZYEXJGOQLDMJ-GEYPSZEHSA-N

Formula: C23H36O3

SMILES: CCCC(=O)OC1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 360.53

Physical Properties

Property code	Value	Unit	Source
gf	-65.34	kJ/mol	Joback Method
hf	-670.69	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	77.48	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.310		Crippen Method
mcvol	300.500	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2702.82		NIST Webbook
tb	904.53	K	Joback Method
tc	1143.14	K	Joback Method
tf	578.59	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.74	J/mol×K	904.53	Joback Method
cpg	1135.18	J/mol×K	944.30	Joback Method
cpg	1163.60	J/mol×K	984.07	Joback Method
cpg	1192.31	J/mol×K	1023.83	Joback Method
cpg	1221.63	J/mol×K	1063.60	Joback Method
cpg	1251.89	J/mol×K	1103.37	Joback Method
cpg	1283.39	J/mol×K	1143.14	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=R190337&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