Epitestosterone, propionate

Inchi: InChI=1S/C22H32O3/c1-4-20(24)25-19-8-7-17-16-6-5-14-13-15(23)9-11-21(14,2)18(16)1
InchiKey: PDMMFKSKQVNJMI-UHFFFAOYSA-N
Formula: C22H32O3
SMILES: CCC(=O)OC1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
gf	-45.72	kJ/mol	Joback Method
hf	-583.40	kJ/mol	Joback Method
hfus	27.45	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.840		Crippen Method
mcvol	282.110	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	890.46	K	Joback Method
tc	1134.37	K	Joback Method
tf	584.84	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.15	J/mol×K	890.46	Joback Method
cpg	1036.22	J/mol×K	931.11	Joback Method
cpg	1063.38	J/mol×K	971.76	Joback Method
cpg	1090.95	J/mol×K	1012.42	Joback Method
cpg	1119.28	J/mol×K	1053.07	Joback Method
cpg	1148.71	J/mol×K	1093.72	Joback Method
cpg	1179.57	J/mol×K	1134.37	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=U368366&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