5«beta»,17«beta»-Dihydrotestosterone propanoate

Inchi: InChI=1S/C21H32O3/c1-3-20(23)24-19-9-8-18-17-6-4-13-12-14(22)5-7-15(13)16(17)10-1

InchiKey: KZOYXNFYEUGSMF-ZZEZVYPVSA-N

Formula: C21H32O3

SMILES: CCC(=O)OC1CCC2C3CCC4CC(=O)CCC4C3CCC12C

Mol. weight [g/mol]: 332.48

Physical Properties

Property code	Value	Unit	Source
gf	-76.69	kJ/mol	Joback Method
hf	-644.65	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	74.18	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.530		Crippen Method
mcvol	272.320	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2677.85		NIST Webbook
rinpol	2690.55		NIST Webbook
rinpol	2677.85		NIST Webbook
tb	858.53	K	Joback Method
tc	1096.95	K	Joback Method
tf	532.15	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.57	J/mol×K	858.53	Joback Method
cpg	1005.45	J/mol×K	898.27	Joback Method
cpg	1029.21	J/mol×K	938.00	Joback Method
cpg	1052.06	J/mol×K	977.74	Joback Method
cpg	1074.20	J/mol×K	1017.47	Joback Method
cpg	1095.82	J/mol×K	1057.21	Joback Method
cpg	1117.12	J/mol×K	1096.95	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=R500091&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