

# 5«alpha»,17«beta»-Dihydrotestosterone 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-MVITVOIJSA-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	2828.20		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/molxK	904.53	Joback Method
cpg	1135.18	J/molxK	944.30	Joback Method
cpg	1163.60	J/molxK	984.07	Joback Method
cpg	1192.31	J/molxK	1023.83	Joback Method
cpg	1221.63	J/molxK	1063.60	Joback Method
cpg	1251.89	J/molxK	1103.37	Joback Method
cpg	1283.39	J/molxK	1143.14	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R190248&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R190248&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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