11«alpha»-Hydroxy-17«alpha»-methyl testosterone

Other names:
4-Androsten-17«alpha»-methyl-11«alpha»,17«beta»-diol-3-one

Androst-4-en-3-one, 11,17-dihydroxy-17-methyl-, (11«alpha»,17«beta»)-

11-Hydroxy-17-methyltestosterone

11Beta-17beta-dihydroxy-17alpha-methylandrost-4-en-3-one

11«alpha»,17«beta»-dihydroxy-17-methylandrost-4-en-3-one

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

InchiKey: UBIBSXMTVJAYTQ-ISQMNYQQSA-N

Formula: C20H30O3

SMILES: CC12CCC(=O)C=C1CCC1C2C(O)CC2(C)C1CCC2(C)O

Mol. weight [g/mol]: 318.45

CAS: 1807-02-9

Physical Properties

Property code	Value	Unit	Source
gf	-115.48	kJ/mol	Joback Method
hf	-606.88	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	94.80	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.240		Crippen Method
mcvol	258.230	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
tb	948.34	K	Joback Method
tc	1178.40	K	Joback Method
tf	631.44	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.00	J/mol×K	948.34	Joback Method
cpg	1012.73	J/mol×K	986.68	Joback Method
cpg	1043.17	J/mol×K	1025.03	Joback Method
cpg	1075.71	J/mol×K	1063.37	Joback Method

cpg	1110.76	J/mol×K	1101.71	Joback Method	
cpg	1148.70	J/mol×K	1140.05	Joback Method	
cpg	1189.93	J/mol×K	1178.40	Joback Method	

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1807029&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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