4-Androsten-3-one, 4,17beta-dihydroxy-17alpha-methyl-

Inchi: InChI=1S/C20H30O3/c1-18-9-8-16(21)17(22)15(18)5-4-12-13(18)6-10-19(2)14(12)7-11-2

InchiKey: RXXBBHGCAXVBES-UHFFFAOYSA-N

Formula: C20H30O3

SMILES: CC12CCC(=O)C(O)=C1CCC1C2CCC2(C)C1CCC2(C)O

Mol. weight [g/mol]: 318.45

CAS: 145841-84-5

Physical Properties

Property code	Value	Unit	Source
gf	-117.40	kJ/mol	Joback Method
hf	-598.01	kJ/mol	Joback Method
hfus	20.97	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.155		Crippen Method
mcvol	258.230	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
tb	957.99	K	Joback Method
tc	1189.14	K	Joback Method
tf	648.20	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.42	J/mol×K	957.99	Joback Method
cpg	1010.66	J/mol×K	996.52	Joback Method
cpg	1041.79	J/mol×K	1035.04	Joback Method
cpg	1075.21	J/mol×K	1073.57	Joback Method
cpg	1111.32	J/mol×K	1112.09	Joback Method
cpg	1150.54	J/mol×K	1150.62	Joback Method
cpg	1193.26	J/mol×K	1189.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C145841845&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:
https://www.chemeo.com/cid/31-175-3/4-Androsten-3-one-4-17beta-dihydroxy-17alpha-methyl.pdf
Generated by Cheméo on 2024-04-20 08:01:44.209102802 +0000 UTC m=+15889353.129680117.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.