Androstan-17-one, 3-hydroxy-, (3«alpha»,5«beta»)-

Other names: 5«beta»-Androstan-17-one, 3«alpha»-hydroxy-
Androsterone, (5«beta»)-
Etiocholan-3«alpha»-ol-17-one
Etiocholanolone
3«alpha»-Etiocholanolone
5«beta»-Androsterone
5-Isoandrosterone
3«alpha»-Hydroxy-5«beta»-androstan-17-one
5«beta»-Androstan-3«alpha»-ol-17-one
3-Hydroxyandrostan-17-one-, (3«alpha»,5«beta»)-
NSC 50908
Ethiocholan-3«alpha»-ol-17-one
5B-Androstan-3A-ol-17-one

Inchi: InChI=1S/C19H30O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14

InchiKey: QGXBDMJGAMFCBF-CYFBJHQBSA-N

Formula: C19H30O2

SMILES: CC12CCC3C(CCC4CC(O)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 290.44

CAS: 53-42-9

Physical Properties

Property code	Value	Unit	Source
gf	-1.92	kJ/mol	Joback Method
hf	-495.56	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.959		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2500.00		NIST Webbook
rinpol	2499.00		NIST Webbook
tb	828.90	K	Joback Method
tc	1062.98	K	Joback Method
tf	522.17	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.61	J/mol×K	828.90	Joback Method
cpg	895.49	J/mol×K	867.91	Joback Method
cpg	920.14	J/mol×K	906.93	Joback Method
cpg	944.87	J/mol×K	945.94	Joback Method
cpg	969.98	J/mol×K	984.95	Joback Method
cpg	995.80	J/mol×K	1023.97	Joback Method
cpg	1022.62	J/mol×K	1062.98	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53429&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume