Androstane-3,17-diol, (3«alpha»,5«alpha»,17«beta»)-

Other names: 5«alpha»-Androstane-3«alpha»,17«beta»-diol
Androstane-3«alpha»,17«beta»-diol
Etiocholane-3«alpha»,17«beta»-diol
Hombreol
3«alpha»,17«beta»-Dihydroxy-5«alpha»-androstane
5«alpha»-Androstane-3«alpha»,17«beta»-androstanediol
(3«alpha»,5«alpha»,17«beta»)-Androstane-3,17-diol
5-alpha-Androstan-3-alpha,17-beta-diol
NSC 9899
5A-Androstan-3A,17B-diol

Inchi: InChI=1S/C19H32O2/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: CBMYJHIOYJEBSB-ZOSDZXSZSA-N

Formula: C19H32O2

SMILES: CC12CCC3C(CCC4CC(O)CCC43C)C1CCC2O

Mol. weight [g/mol]: 292.46

CAS: 1852-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-23.86	kJ/mol	Joback Method
hf	-530.43	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	88.22	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.751		Crippen Method
mcvol	246.870	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	848.59	K	Joback Method
tc	1062.44	K	Joback Method
tf	510.53	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.30	J/mol×K	848.59	Joback Method
cpg	930.23	J/mol×K	884.23	Joback Method
cpg	953.16	J/mol×K	919.87	Joback Method
cpg	976.35	J/mol×K	955.52	Joback Method
cpg	1000.05	J/mol×K	991.16	Joback Method
cpg	1024.53	J/mol×K	1026.80	Joback Method
cpg	1050.06	J/mol×K	1062.44	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1852535&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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