

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

Other names:	Androst-5-ene-3«beta»,17«alpha»-diol «delta»5-Androsten-3«beta»,17«alpha»-diol Androst-5-en-3«beta»,17«alpha»-diol 3«beta»,17«alpha»-Dihydroxy-androst-5-ene 3«beta»,17«alpha»-Androst-5-ene-3,17-diol Androst-5-en-3-beta,17-alpha-diol Androst-5-en-3B,17A-diol
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:	QADHLRWLCPCEKT-UHFFFAOYSA-N
Formula:	C19H30O2
SMILES:	CC12CCC(O)CC1=CCC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]:	290.44
CAS:	1963-03-7

Physical Properties

Property code	Value	Unit	Source
gf	4.18	kJ/mol	Joback Method
hf	-463.78	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	89.48	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.671		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
tb	857.40	K	Joback Method
tc	1073.36	K	Joback Method
tf	528.05	K	Joback Method
vc	0.904	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.45	J/mol×K	857.40	Joback Method
cpg	897.54	J/mol×K	893.39	Joback Method

cpg	919.80	J/mol×K	929.39	Joback Method
cpg	942.52	J/mol×K	965.38	Joback Method
cpg	965.95	J/mol×K	1001.38	Joback Method
cpg	990.39	J/mol×K	1037.37	Joback Method
cpg	1016.09	J/mol×K	1073.36	Joback Method

Sources

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=C1963037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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