Androst-16-en-3-one, (5«alpha»)-

Other names:	5«alpha»-Androst-16-en-3-one
	Androst-16-en-3-one
	5«alpha»-Androstenone
	Androstenone
Inchi:	InChI=1S/C19H28O/c1-18-9-3-4-16(18)15-6-5-13-12-14(20)7-11-19(13,2)17(15)8-10-18/
InchiKey:	HFVMLYAGWXSTQI-NKOUSSCVSA-N
Formula:	C19H28O
SMILES:	CC12C=CCC1C1CCC3CC(=O)CCC3(C)C1CC2
Mol. weight [g/mol]:	272.43
CAS:	18339-16-7

Physical Properties

Property code	Value	Unit	Source
gf	172.57	kJ/mol	Joback Method
hf	-265.21	kJ/mol	Joback Method
hfus	17.28	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.764		Crippen Method
mcvol	232.400	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
ripol	2160.00		NIST Webbook
tb	740.55	K	Joback Method
tc	997.16	K	Joback Method
tf	466.35	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.73	J/mol×K	740.55	Joback Method
cpg	790.96	J/mol×K	783.32	Joback Method
cpg	817.25	J/mol×K	826.09	Joback Method
cpg	843.02	J/mol×K	868.86	Joback Method

cpg	868.69	J/mol×K	911.62	Joback Method
cpg	894.67	J/mol×K	954.39	Joback Method
cpg	921.40	J/mol×K	997.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18339167&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume