Androstenedione

Other names:	3,17-Dioxoandrost-4-ene
	4-Androsten-3,17-dione
	4-Androsten-3,7-dione
	4-Androstene-3,17-dione
	Androstenedione AS 181
	NSC 9563
	SKF 2170
	androst-4-ene-3,17-dione
	«delta»(Sup4)-Androstene-3,17-dione
	«delta»-(sup4)-Androsten-3,17-dione
	«delta»4-Androsten-3,17-dione
	«delta»4-Androstene-3,17-dione
Inchi:	InChI=1S/C19H26O2/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:	AEMFNILZOJDQLW-JRCHKSGSSA-N
Formula:	C19H26O2
SMILES:	CC12CCC3C(CCC4=CC(=O)CCC43C)C1CCC2=O
Mol. weight [g/mol]:	286.41
CAS:	63-05-8

Physical Properties

Property code	Value	Unit	Source
chs	-10760.00 ± 30.00	kJ/mol	NIST Webbook
gf	48.06	kJ/mol	Joback Method
hf	-394.04	kJ/mol	Joback Method
hfus	25.70	kJ/mol	Solubility of androstenedione in lower alcohols
hvap	65.24	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.087		Crippen Method
mcvol	233.970	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2497.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	818.02	K	Joback Method
tc	1084.47	K	Joback Method

tf	551.33	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.48	J/mol×K	818.02	Joback Method
cpg	830.12	J/mol×K	862.43	Joback Method
cpg	856.47	J/mol×K	906.84	Joback Method
cpg	882.94	J/mol×K	951.24	Joback Method
cpg	909.95	J/mol×K	995.65	Joback Method
cpg	937.91	J/mol×K	1040.06	Joback Method
cpg	967.22	J/mol×K	1084.47	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=C63058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of androstenedione in lower alcohols:	https://www.doi.org/10.1016/j.fluid.2013.11.008

Legend

chs:	Standard solid enthalpy of combustion
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