Androst-1-ene-3,17-dione, (5«alpha»)-

Other names: 5«alpha»-Androst-1-ene-3,17-dione
«delta»1-5«alpha»-Androstene-3,17-dione
5alpha-Androst-1-ene-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: WJIQCDPCDVWDDE-UHFFFAOYSA-N
Formula: C19H26O2
SMILES: CC12CCC3C(CCC4CC(=O)C=CC43C)C1CCC2=O
Mol. weight [g/mol]: 286.41
CAS: 571-40-4

Physical Properties

Property code	Value	Unit	Source
gf	49.98	kJ/mol	Joback Method
hf	-402.91	kJ/mol	Joback Method
hfus	16.79	kJ/mol	Joback Method
hvap	64.27	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.943		Crippen Method
mcvol	233.970	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
tb	808.37	K	Joback Method
tc	1074.47	K	Joback Method
tf	534.57	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.58	J/mol×K	808.37	Joback Method
cpg	833.61	J/mol×K	852.72	Joback Method
cpg	860.17	J/mol×K	897.07	Joback Method
cpg	886.69	J/mol×K	941.42	Joback Method
cpg	913.57	J/mol×K	985.77	Joback Method
cpg	941.22	J/mol×K	1030.12	Joback Method

cpg	970.05	J/mol×K	1074.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C571404&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume