

Androst-4-ene-3,17-dione, 19-hydroxy-

Other names:	19-Hydroxy-4-androstene-3,17-dione 19-Hydroxyandrost-4-ene-3,17-dione
Inchi:	InChI=1S/C19H26O3/c1-18-8-7-16-14(15(18)4-5-17(18)22)3-2-12-10-13(21)6-9-19(12,16)
InchiKey:	XGUHPTGEXRHMQQ-UHFFFAOYSA-N
Formula:	C19H26O3
SMILES:	CC12CCC3C(CCC4=CC(=O)CCC43CO)C1CCC2=O
Mol. weight [g/mol]:	302.41
CAS:	510-64-5

Physical Properties

Property code	Value	Unit	Source
gf	-88.76	kJ/mol	Joback Method
hf	-546.27	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.060		Crippen Method
mcvol	239.840	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
tb	910.20	K	Joback Method
tc	1155.76	K	Joback Method
tf	612.15	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.89	J/mol×K	910.20	Joback Method
cpg	901.41	J/mol×K	951.13	Joback Method
cpg	926.38	J/mol×K	992.05	Joback Method
cpg	952.13	J/mol×K	1032.98	Joback Method
cpg	978.97	J/mol×K	1073.91	Joback Method
cpg	1007.24	J/mol×K	1114.84	Joback Method
cpg	1037.25	J/mol×K	1155.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C510645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	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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