

Androst-4-en-3-one, 17-hydroxy-, (17«alpha»)-

Other names:	Androst-4-en-3-one, 17«alpha»-hydroxy- cis-Testosterone Epitestosterone Isotestosterone Testosterone, cis- 17«alpha»-Hydroxyandrost-4-en-3-one 17«alpha»-Testosterone 17-Epitestosterone 4-Androsten-17«alpha»-ol-3-one 17-Hydroxyandrost-4-en-3-one, (17«alpha»)- 17alpha-Hydroxyandrost-4-en-3-one NSC 26499
Inchi:	InChI=1S/C19H28O2/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:	MUMGGOZAMZWBJJ-YDJBQETSA-N
Formula:	C19H28O2
SMILES:	CC12CCC(=O)C=C1CCC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]:	288.42
CAS:	481-30-1

Physical Properties

Property code	Value	Unit	Source
gf	26.12	kJ/mol	Joback Method
hf	-428.91	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	77.36	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.879		Crippen Method
mcvol	238.270	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	2729.20		NIST Webbook
tb	837.71	K	Joback Method
tc	1074.12	K	Joback Method
tf	539.69	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.35	J/mol×K	837.71	Joback Method
cpg	863.19	J/mol×K	877.11	Joback Method
cpg	887.01	J/mol×K	916.51	Joback Method
cpg	911.12	J/mol×K	955.91	Joback Method
cpg	935.84	J/mol×K	995.32	Joback Method
cpg	961.51	J/mol×K	1034.72	Joback Method
cpg	988.44	J/mol×K	1074.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C481301&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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