Estr-4-en-3-one, 17«alpha»-hydroxy-17-methyl-

Other names: 17«beta»-Methyl-19-nortestosterone
17«alpha»-Hydroxy-17-methylestr-4-en-3-one
17Alpha-methyl-beta-nortestosterone

Inchi: InChI=1S/C19H28O2/c1-18-9-7-15-14-6-4-13(20)11-12(14)3-5-16(15)17(18)8-10-19(18,2

InchiKey: ZXSWTMLNIIZPET-UHFFFAOYSA-N

Formula: C19H28O2

SMILES: CC1(O)CCC2C3CCC4=CC(=O)CCC4C3CCC21C

Mol. weight [g/mol]: 288.42

CAS: 10582-09-9

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
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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10582099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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