

Epitestosterone, formate

Inchi:	InChI=1S/C20H28O3/c1-19-9-7-14(22)11-13(19)3-4-15-16-5-6-18(23-12-21)20(16,2)10-8
InchiKey:	LMUMOFOWZKACOU-UHFFFAOYSA-N
Formula:	C20H28O3
SMILES:	CC12CCC(=O)C=C1CCC1C2CCC2(C)C(OC=O)CCC12
Mol. weight [g/mol]:	316.43

Physical Properties

Property code	Value	Unit	Source
gf	-33.16	kJ/mol	Joback Method
hf	-515.12	kJ/mol	Joback Method
hfus	22.96	kJ/mol	Joback Method
hvap	72.04	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.060		Crippen Method
mcvol	253.930	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinsol	2404.00		NIST Webbook
tb	839.49	K	Joback Method
tc	1087.32	K	Joback Method
tf	554.37	K	Joback Method
vc	0.966	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.70	J/mol×K	839.49	Joback Method
cpg	907.20	J/mol×K	880.79	Joback Method
cpg	932.52	J/mol×K	922.10	Joback Method
cpg	958.02	J/mol×K	963.40	Joback Method
cpg	984.04	J/mol×K	1004.71	Joback Method
cpg	1010.95	J/mol×K	1046.01	Joback Method
cpg	1039.07	J/mol×K	1087.32	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=U368365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
mccol:	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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