17-«beta»-Methyl-5-«beta»-androstan-3-«beta»,17

Inchi: InChI=1S/C20H34O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(1
InchiKey: QGKQXZFZOIQFBI-QPPSVRFASA-N
Formula: C20H34O2
SMILES: CC12CCC(O)CC1CCC1C2CCC2(C)C1CCC2(C)O
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	-20.93	kJ/mol	Joback Method
hf	-535.83	kJ/mol	Joback Method
hfus	23.16	kJ/mol	Joback Method
hvap	89.30	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.141		Crippen Method
mcvol	260.960	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	2527.00		NIST Webbook
tb	871.71	K	Joback Method
tc	1089.20	K	Joback Method
tf	545.70	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.80	J/mol×K	871.71	Joback Method
cpg	993.94	J/mol×K	907.96	Joback Method
cpg	1020.92	J/mol×K	944.21	Joback Method
cpg	1049.12	J/mol×K	980.46	Joback Method
cpg	1078.90	J/mol×K	1016.70	Joback Method
cpg	1110.63	J/mol×K	1052.95	Joback Method
cpg	1144.66	J/mol×K	1089.20	Joback Method

Sources

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=R257564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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