17-epi-Methandriol

Inchi: InChI=1S/C20H32O2/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: WRWBCPJQPDHXTJ-RZNHXTIWSA-N
Formula: C20H32O2
SMILES: CC12CCC(O)CC1=CCC1C2CCC2(C)C1CCC2(C)O
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	7.11	kJ/mol	Joback Method
hf	-469.18	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	90.56	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.061		Crippen Method
mcvol	256.660	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2562.00		NIST Webbook
rinpol	2562.00		NIST Webbook
tb	880.52	K	Joback Method
tc	1100.10	K	Joback Method
tf	563.22	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.87	J/mol×K	880.52	Joback Method
cpg	961.45	J/mol×K	917.12	Joback Method
cpg	988.11	J/mol×K	953.71	Joback Method
cpg	1016.23	J/mol×K	990.31	Joback Method
cpg	1046.18	J/mol×K	1026.91	Joback Method
cpg	1078.34	J/mol×K	1063.51	Joback Method
cpg	1113.10	J/mol×K	1100.10	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=R257831&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume