3«beta»-hydroxy-manoyl oxide isomer

Inchi: InChI=1S/C20H34O2/c1-7-18(4)11-8-15-19(5)12-10-16(21)17(2,3)14(19)9-13-20(15,6)22
InchiKey: JJZSRKRSWWPWCJ-MUAWJZPLSA-N
Formula: C20H34O2
SMILES: C=CC1(C)CCC2C(C)(CCC3C(C)(C)C(O)CCC23C)O1
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	51.37	kJ/mol	Joback Method
hf	-447.73	kJ/mol	Joback Method
hfus	21.34	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.714		Crippen Method
mcvol	267.520	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	796.66	K	Joback Method
tc	1020.68	K	Joback Method
tf	515.65	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.29	J/mol×K	796.66	Joback Method
cpg	932.72	J/mol×K	834.00	Joback Method
cpg	959.84	J/mol×K	871.33	Joback Method
cpg	988.09	J/mol×K	908.67	Joback Method
cpg	1017.95	J/mol×K	946.01	Joback Method
cpg	1049.87	J/mol×K	983.35	Joback Method
cpg	1084.31	J/mol×K	1020.68	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=R333470&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