7«alpha»-hydroxymanool

Inchi: InChI=1S/C20H34O2/c1-7-19(5,22)11-10-15-12-17(21)18(3,4)16-9-8-14(2)13-20(15,16)6
InchiKey: QBGCJSNIPHJJCV-AZDWTMOSSA-N
Formula: C20H34O2
SMILES: C=CC(C)(O)CCC1CC(O)C(C)(C)C2CCC(=C)CC12C
Mol. weight [g/mol]: 306.48

Physical Properties

Property code	Value	Unit	Source
gf	26.63	kJ/mol	Joback Method
hf	-469.25	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	88.95	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.473		Crippen Method
mcvol	274.080	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	851.00	K	Joback Method
tc	1054.41	K	Joback Method
tf	508.02	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.83	J/mol×K	851.00	Joback Method
cpg	957.92	J/mol×K	884.90	Joback Method
cpg	979.01	J/mol×K	918.80	Joback Method
cpg	1000.30	J/mol×K	952.71	Joback Method
cpg	1022.02	J/mol×K	986.61	Joback Method
cpg	1044.37	J/mol×K	1020.51	Joback Method
cpg	1067.56	J/mol×K	1054.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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