(+)-(1R*,4S*,5S*,7S*,10S*)-viticulol

Inchi: InChI=1S/C20H34O/c1-14(2)7-6-8-15(3)17-11-12-20(5,21)19-10-9-16(4)18(19)13-17/h7,
InchiKey: DOGQNYXCCXBVMX-UILHHMQZSA-N
Formula: C20H34O
SMILES: C=C(CCC=C(C)C)C1CCC(C)(O)C2CCC(C)C2C1
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	176.14	kJ/mol	Joback Method
hf	-310.11	kJ/mol	Joback Method
hfus	32.73	kJ/mol	Joback Method
hvap	74.68	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.502		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
tb	766.57	K	Joback Method
tc	970.29	K	Joback Method
tf	374.20	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.85	J/mol×K	766.57	Joback Method
cpg	887.94	J/mol×K	800.52	Joback Method
cpg	909.13	J/mol×K	834.48	Joback Method
cpg	929.56	J/mol×K	868.43	Joback Method
cpg	949.36	J/mol×K	902.38	Joback Method
cpg	968.68	J/mol×K	936.34	Joback Method
cpg	987.65	J/mol×K	970.29	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=R406385&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