Vomifoliol

Inchi: InChI=1S/C12H18O3/c1-9(13)4-6-12(15)7-5-10(14)8-11(12,2)3/h4-7,9,13,15H,8H2,1-3H
InchiKey: BZYRKOLLJAWIFZ-KFFBJUEBSA-N
Formula: C12H18O3
SMILES: CC(O)C=CC1(O)C=CC(=O)CC1(C)C
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-232.57	kJ/mol	Joback Method
hf	-498.99	kJ/mol	Joback Method
hfus	12.73	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.210		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
tb	744.38	K	Joback Method
tc	951.91	K	Joback Method
tf	446.48	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.79	J/mol×K	744.38	Joback Method
cpg	527.61	J/mol×K	778.97	Joback Method
cpg	541.30	J/mol×K	813.56	Joback Method
cpg	555.03	J/mol×K	848.14	Joback Method
cpg	568.96	J/mol×K	882.73	Joback Method
cpg	583.27	J/mol×K	917.32	Joback Method
cpg	598.11	J/mol×K	951.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R614749&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