1,8-Dihydrovomifoliol

Other names: 7,8-dihydrovomifoliol
Inchi: InChI=1S/C13H22O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h7,10,14,16H,5-6,8H2,
InchiKey: CWOFGGNDZOPNFG-GWCFXTLKSA-N
Formula: C13H22O3
SMILES: CC1=CC(=O)CC(C)(C)C1(O)CCC(C)O
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-314.00	kJ/mol	Joback Method
hf	-648.32	kJ/mol	Joback Method
hfus	14.73	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.824		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
ripol	3262.00		NIST Webbook
tb	768.08	K	Joback Method
tc	968.62	K	Joback Method
tf	475.35	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.30	J/mol×K	768.08	Joback Method
cpg	607.40	J/mol×K	801.50	Joback Method
cpg	622.37	J/mol×K	834.93	Joback Method
cpg	637.35	J/mol×K	868.35	Joback Method
cpg	652.48	J/mol×K	901.77	Joback Method
cpg	667.89	J/mol×K	935.19	Joback Method
cpg	683.71	J/mol×K	968.62	Joback Method

Sources

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=R231651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume