3,4-dihydro-«gamma»-ionol

Inchi: InChI=1S/C13H24O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h7-8,10-12,14H,5-6,9H2,1-4H
InchiKey: CGAOOLUOEOTNNY-BQYQJAHWSA-N
Formula: C13H24O
SMILES: CC(O)C=CC1C(C)CCCC1(C)C
Mol. weight [g/mol]: 196.33

Physical Properties

Property code	Value	Unit	Source
gf	3.08	kJ/mol	Joback Method
hf	-323.06	kJ/mol	Joback Method
hfus	17.87	kJ/mol	Joback Method
hvap	59.44	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.386		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
tb	603.19	K	Joback Method
tc	800.30	K	Joback Method
tf	299.81	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.71	J/mol×K	603.19	Joback Method
cpg	521.25	J/mol×K	636.04	Joback Method
cpg	538.83	J/mol×K	668.89	Joback Method
cpg	555.56	J/mol×K	701.75	Joback Method
cpg	571.52	J/mol×K	734.60	Joback Method
cpg	586.82	J/mol×K	767.45	Joback Method
cpg	601.55	J/mol×K	800.30	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=R279440&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