dihydro- «gamma»-ionol

Inchi: InChI=1S/C13H24O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h11-12,14H,1,5-9H2,2-4H3
InchiKey: XYSOCYCFJHMQON-UHFFFAOYSA-N
Formula: C13H24O
SMILES: C=C1CCCC(C)(C)C1CCC(C)O
Mol. weight [g/mol]: 196.33

Physical Properties

Property code	Value	Unit	Source
gf	-16.35	kJ/mol	Joback Method
hf	-335.70	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	59.95	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.530		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
ripol	1935.00		NIST Webbook
ripol	1935.00		NIST Webbook
tb	602.86	K	Joback Method
tc	794.02	K	Joback Method
tf	322.81	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.44	J/mol×K	602.86	Joback Method
cpg	516.90	J/mol×K	634.72	Joback Method
cpg	533.52	J/mol×K	666.58	Joback Method
cpg	549.38	J/mol×K	698.44	Joback Method
cpg	564.54	J/mol×K	730.30	Joback Method
cpg	579.10	J/mol×K	762.16	Joback Method
cpg	593.13	J/mol×K	794.02	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=R344168&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume