5-Oxo-dihydro- «alpha»-ionol

Inchi: InChI=1S/C13H24O2/c1-10(14)6-7-11-12(2,3)8-5-9-13(11,4)15/h6-7,10-11,14-15H,5,8-9H
InchiKey: JISIFGMVPLRJDQ-VOTSOKGWSA-N
Formula: C13H24O2
SMILES: CC(O)C=CC1C(C)(C)CCCC1(C)O
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-139.23	kJ/mol	Joback Method
hf	-460.05	kJ/mol	Joback Method
hfus	15.66	kJ/mol	Joback Method
hvap	74.97	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.501		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
ripol	2709.00		NIST Webbook
ripol	2709.00		NIST Webbook
tb	695.61	K	Joback Method
tc	888.91	K	Joback Method
tf	384.53	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.68	J/mol×K	695.61	Joback Method
cpg	581.23	J/mol×K	727.83	Joback Method
cpg	596.34	J/mol×K	760.04	Joback Method
cpg	611.17	J/mol×K	792.26	Joback Method
cpg	625.87	J/mol×K	824.48	Joback Method
cpg	640.60	J/mol×K	856.69	Joback Method
cpg	655.50	J/mol×K	888.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R344608&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume