(E)-3-Oxo-retro-«alpha»-ionol

Inchi: InChI=1S/C13H22O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h6,9-10,14H,5,7-8H2,1-4H
InchiKey: PEEBQRPOLIDAGI-WUXMJOGZSA-N
Formula: C13H22O2
SMILES: CC(O)CC=C1C(C)CC(=O)CC1(C)C
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-146.56	kJ/mol	Joback Method
hf	-481.61	kJ/mol	Joback Method
hfus	16.43	kJ/mol	Joback Method
hvap	64.83	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.709		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1693.00		NIST Webbook
rinpol	1692.00		NIST Webbook
tb	678.16	K	Joback Method
tc	884.96	K	Joback Method
tf	387.71	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.94	J/mol×K	678.16	Joback Method
cpg	552.98	J/mol×K	712.63	Joback Method
cpg	569.28	J/mol×K	747.09	Joback Method
cpg	584.91	J/mol×K	781.56	Joback Method
cpg	599.94	J/mol×K	816.03	Joback Method
cpg	614.46	J/mol×K	850.49	Joback Method
cpg	628.55	J/mol×K	884.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R230049&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