Retro-ionone

Inchi: InChI=1S/C13H22O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h8,10H,5-7,9H2,1-4H3/b12-8-
InchiKey: DTATXKHAJFDHQB-XYOKQWHBSA-N
Formula: C13H22O
SMILES: CC(=O)CC=C1C(C)CCCC1(C)C
Mol. weight [g/mol]: 194.31

Physical Properties

Property code	Value	Unit	Source
gf	-13.63	kJ/mol	Joback Method
hf	-298.98	kJ/mol	Joback Method
hfus	17.96	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.738		Crippen Method
mcvol	180.440	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
tb	572.47	K	Joback Method
tc	784.82	K	Joback Method
tf	323.60	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.89	J/mol×K	572.47	Joback Method
cpg	477.29	J/mol×K	607.86	Joback Method
cpg	495.60	J/mol×K	643.25	Joback Method
cpg	512.93	J/mol×K	678.65	Joback Method
cpg	529.40	J/mol×K	714.04	Joback Method
cpg	545.10	J/mol×K	749.43	Joback Method
cpg	560.15	J/mol×K	784.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R635662&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