Methyl ionone 3

Inchi: InChI=1S/C14H22O/c1-5-12(15)8-9-13-11(2)7-6-10-14(13,3)4/h7-9,13H,5-6,10H2,1-4H3
InchiKey: VPKMGDRERYMTJX-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CCC(=O)C=CC1C(C)=CCCC1(C)C
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	49.88	kJ/mol	Joback Method
hf	-232.12	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	53.38	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1530.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1930.00		NIST Webbook
tb	597.01	K	Joback Method
tc	811.30	K	Joback Method
tf	332.71	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.29	J/mol×K	597.01	Joback Method
cpg	508.42	J/mol×K	632.73	Joback Method
cpg	526.47	J/mol×K	668.44	Joback Method
cpg	543.56	J/mol×K	704.16	Joback Method
cpg	559.82	J/mol×K	739.87	Joback Method
cpg	575.38	J/mol×K	775.59	Joback Method
cpg	590.35	J/mol×K	811.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410007&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume