Methyl ionone I

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

Physical Properties

Property code	Value	Unit	Source
gf	41.33	kJ/mol	Joback Method
hf	-241.91	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	53.46	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
ripol	1836.00		NIST Webbook
ripol	1836.00		NIST Webbook
tb	596.89	K	Joback Method
tc	814.96	K	Joback Method
tf	318.75	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.05	J/mol×K	596.89	Joback Method
cpg	508.48	J/mol×K	633.24	Joback Method
cpg	526.79	J/mol×K	669.58	Joback Method
cpg	544.12	J/mol×K	705.93	Joback Method
cpg	560.60	J/mol×K	742.27	Joback Method
cpg	576.37	J/mol×K	778.62	Joback Method

cpg	591.55	J/mol×K	814.96	Joback Method

Sources

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=R410027&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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