«alpha»-Irone

Other names:	3-Buten-2-one, 4-(2,5,6,6-tetramethyl-2-cyclohexen-1-yl)-
	«alpha»-Ionone, 6-methyl-
	Methyl-«alpha»-ionone
	6-Methyl-«alpha»-ionone
	«alpha»-Methyl-ionone
	Ionone 6-Methyl, «alpha»
	4-(2,5,6,6-Tetramethyl-2-cyclohexen-1-yl)-3-buten-2-one
	«alpha»-Ionone, methyl-
	4-(2,5,6,6-tetramethylcyclohex-2-enyl)but-3-en-2-one
Inchi:	InChI=1S/C14H22O/c1-10-6-7-11(2)14(4,5)13(10)9-8-12(3)15/h6,8-9,11,13H,7H2,1-5H3/
InchiKey:	JZQOJFLIJNRDHK-MDQMCFMNSA-N
Formula:	C14H22O
SMILES:	CC(=O)C=CC1C(C)=CCC(C)C1(C)C
Mol. weight [g/mol]:	206.32
CAS:	79-69-6

Physical Properties

Property code	Value	Unit	Source
gf	42.17	kJ/mol	Joback Method
hf	-252.46	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hvap	53.08	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.760		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1519.00		NIST Webbook
ripol	2068.00		NIST Webbook
ripol	2068.00		NIST Webbook
tb	592.34	K	Joback Method

tc	806.59	K	Joback Method
tf	328.47	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.54	J/mol×K	592.34	Joback Method
cpg	510.15	J/mol×K	628.05	Joback Method
cpg	528.68	J/mol×K	663.76	Joback Method
cpg	546.23	J/mol×K	699.46	Joback Method
cpg	562.93	J/mol×K	735.17	Joback Method
cpg	578.89	J/mol×K	770.88	Joback Method
cpg	594.23	J/mol×K	806.59	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79696&Units=SI

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