«alpha» Isomethyl ionone

Other names:	4-(2,6,6-Trimethyl 2-cyclohexen-1-yl)-3-methyl-3-buten-2-one
	3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
	«alpha»-Cetone
	«alpha»-Ionone, isomethyl-
	Cetone alpha
	iso-«alpha»-methyl ionone
	Isomethyl-«alpha»-ionone
	Methyl-«alpha»-isoionone
	8-Methyl-«alpha»-ionone
	NSC 66432
	3-methyl-4-(2,6,6-trimethyl-2-cyclohexenyl)-3-buten-2-one
	3-Methyl-4-(2,6,6-trimethylcyclohex-2-enyl)-but-3-en-2-one
	3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
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/b1
InchiKey:	JRJBVWJSTHECJK-PKNBQFBNSA-N
Formula:	C14H22O
SMILES:	CC(=O)C(C)=CC1C(C)=CCCC1(C)C
Mol. weight [g/mol]:	206.32
CAS:	127-51-5

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	1482.00		NIST Webbook
rinpol	1471.80		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1484.50		NIST Webbook
rinpol	1473.00		NIST Webbook

rinpol	1471.80		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1473.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1877.00		NIST Webbook
ripol	1848.00		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	576.37	J/mol×K	778.62	Joback Method
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	591.55	J/mol×K	814.96	Joback Method
hvapt	69.50	kJ/mol	310.50	NIST Webbook

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=C127515&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
hvapt:	Enthalpy of vaporization at a given temperature
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