

«gamma»-Methylionone

Other names:	4-(2,2-dimethyl-6-methylenecyclohexyl)but-3-en-2-one, monomethyl derivative
Inchi:	InChI=1S/C14H22O/c1-5-12(15)8-9-13-11(2)7-6-10-14(13,3)4/h8-9,13H,2,5-7,10H2,1,3-4H
InchiKey:	VBPVRSYPVFNWFV-CMDGGOBGSA-N
Formula:	C14H22O
SMILES:	C=C1CCCC(C)(C)C1C=CC(=O)CC
Mol. weight [g/mol]:	206.32
CAS:	27417-37-4

Physical Properties

Property code	Value	Unit	Source
gf	82.63	kJ/mol	Joback Method
hf	-194.19	kJ/mol	Joback Method
hfus	19.27	kJ/mol	Joback Method
hvap	52.59	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	592.03	K	Joback Method
tc	805.16	K	Joback Method
tf	333.11	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.23	J/mol×K	592.03	Joback Method
cpg	507.56	J/mol×K	627.55	Joback Method
cpg	525.80	J/mol×K	663.07	Joback Method
cpg	543.06	J/mol×K	698.59	Joback Method
cpg	559.47	J/mol×K	734.12	Joback Method

cpg	575.14	J/mol×K	769.64	Joback Method
cpg	590.20	J/mol×K	805.16	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=C27417374&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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