4-Acetyl-1-methylcyclohexene

Other names:	4-Acetyl-1-methyl-1-cyclohexene
	Ethanone, 1-(4-methyl-3-cyclohexen-1-yl)-
	1-(4-Methyl-3-cyclohexen-1-yl)ethanone
	1-Methyl-4-acetylcyclohex-1-ene
	4-Acetyl-1-methylcyclohex-1-ene
	Cyclohexene, 1-methyl-4-acetyl
	Cyclohexene, 4-acetyl-1-methyl
	Ketone, methyl 4-methyl-3-cyclohexen-1-yl
	Methyl 4-methyl-3-cyclohexen-1-yl ketone
	Limona ketone
	4-Methyl-3-cyclohexen-1-yl methyl ketone
Inchi:	InChI=1S/C9H14O/c1-7-3-5-9(6-4-7)8(2)10/h3,9H,4-6H2,1-2H3
InchiKey:	HOBBEYSRFFJETF-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC(=O)C1CC=C(C)CC1
Mol. weight [g/mol]:	138.21
CAS:	6090-09-1

Physical Properties

Property code	Value	Unit	Source
gf	-59.24	kJ/mol	Joback Method
hf	-241.04	kJ/mol	Joback Method
hfus	13.33	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1147.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1131.20		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook

ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	482.88	K	Joback Method
tc	696.61	K	Joback Method
tf	261.78	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.91	J/mol×K	482.88	Joback Method
cpg	282.78	J/mol×K	518.50	Joback Method
cpg	297.81	J/mol×K	554.12	Joback Method
cpg	312.02	J/mol×K	589.75	Joback Method
cpg	325.44	J/mol×K	625.37	Joback Method
cpg	338.08	J/mol×K	660.99	Joback Method
cpg	349.96	J/mol×K	696.61	Joback Method
dvisc	0.0032877	Pa×s	261.78	Joback Method
dvisc	0.0017144	Pa×s	298.63	Joback Method
dvisc	0.0010315	Pa×s	335.48	Joback Method
dvisc	0.0006862	Pa×s	372.33	Joback Method
dvisc	0.0004913	Pa×s	409.18	Joback Method
dvisc	0.0003717	Pa×s	446.03	Joback Method
dvisc	0.0002935	Pa×s	482.88	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=C6090091&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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